

# Technical Report # KU-EC-12-1: New Cell-Specific and Overall Tests of Spatial Interaction Based on Nearest Neighbor Contingency Tables

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March 7, 2013

## Abstract

Spatial interaction patterns such as segregation and association can be tested using nearest neighbor contingency tables (NNCTs). We introduce new cell-specific (or pairwise) and overall segregation tests and determine their asymptotic distributions. In particular, we demonstrate that cell-specific tests enjoy asymptotic normality, while overall tests have chi-square distributions asymptotically. We also perform an extensive Monte Carlo simulation study to compare the finite sample performance of the tests in terms of empirical size and power. In addition to the cell-specific tests as post-hoc tests for overall tests, we discuss one-class-versus-rest type of NNCT-tests after an overall test yields significant interaction. We also introduce the concepts of total, strong, and partial segregation/association to label levels of these patterns. We compare these new tests with the existing NNCT-tests in literature with simulations as well and illustrate the NNCT-tests on an ecological data set.

*Keywords:* Association; completely mapped data; complete spatial randomness; random labeling; segregation

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## 1 Introduction

Multivariate clustering patterns such as segregation and association result from multivariate interaction between two or more classes (or species). For convenience, categories of the points or units are referred to as “classes”, e.g., a class can stand for species, sex, or some other characteristic of the unit/subject. Segregation is the spatial pattern in which points from the same class are closer to each other, while association is the pattern in which points from different classes are closer to each other. These patterns may have important implications in ecology, plant biology, or epidemiology. See, for example, Whipple (1980), Diggle (2003), and Hamill and Wright (1986). In particular, in ecology, two tree species could be highly dependent on each other (as a result of, say, symbiosis or mutualism), and thus, coexist in a close vicinity (i.e., they are associated), or they could be enjoying the company of conspecifics and so form one-class clumps or groups (i.e., they are segregated). In epidemiology, cases might be clustered compared to controls, due to infectious nature of a disease or closeness to a source of the disease (i.e., cases and controls are segregated). In a social context, segregation of residences due to the socioeconomic status or ethnicity can be investigated by generative models (Fossett (2011)). In literature, spatial segregation is also used to refer to a univariate pattern of spatial clustering (Robertson and Cushing (2011)), which is referred to as aggregation (Ceyhan (2008)). In a social network, segregation of individuals are also modeled via random graph theoretical tools (Henry et al. (2011)). In veterinary epidemiology, a nonparametric method for detecting spatial segregation according to the genotype and year of occurrence of bovine tuberculosis is employed by Diggle et al. (2005).

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Many (univariate or multivariate) spatial clustering tests are proposed in literature (see Kulldorff (2006) for an extensive review). These methods include Ripley’s  $K$ -function (Ripley (2004)), or  $J$ -function (van Lieshout and Baddeley (1999)), nearest neighbor (NN) methods (Diggle (2003)) and so on. Among NN methods, this article concerns the nearest neighbor contingency tables (NNCTs). Pielou (1961) introduced various tests based on NNCTs, however, Dixon (1994) extended these tests in various directions, and also determined the correct asymptotic distribution of the proposed tests. Ceyhan (2008, 2009) compared NNCT-tests in literature, and also proposed various tests based on NNCTs.

In this article, we introduce various new cell-specific segregation tests and overall tests based on these cell-specific tests. We compare these tests with the existing NNCT-tests in literature (Dixon (1994, 2002), Ceyhan (2010)). We demonstrate that cell-specific tests are asymptotically normal, and overall tests tend to chi-square tests with the corresponding degrees of freedom. In practice, cell-specific tests serve as post-hoc tests to be performed when an overall test yields a significant result. As an alternative post-hoc test after a significant overall test, we discuss one-class-versus-rest type of NNCT-tests. By extensive simulations, we compare the newly proposed tests to the ones in literature in terms of empirical size and power, and so demonstrate that one type of the new cell-specific tests and overall tests perform better compared to other tests.

We describe the NNCTs and provide the null and alternative patterns in Section 2, provide the cell-specific tests in Section 3, overall tests in Section 4, empirical significance levels in the two- and three-class cases in Sections 5 and 6, respectively, and empirical power analysis under segregation and association in the two-class and three-class cases in Sections 7 and 8, respectively. We present the empirical size and power analysis for the one-vs-rest type testing in the three-class case in Section 9, the illustration on the example data set in Section 10, and our conclusions and guidelines for using the tests in Section 11.

## 2 Null and Alternative Spatial Patterns and NNCTs

We describe the spatial point patterns for two classes only; the extension to multi-class case is straightforward. Our null hypothesis is

$$H_o : \text{randomness in the NN structure}$$

which may result from random labeling (RL) or independence of points from two classes. Under independence, the two classes result independently from the same stochastic process, hence their spatial distribution is identical. In this article, among independence patterns we will only consider complete spatial randomness (CSR) of points from two classes. Roughly, under CSR independence, two classes are independently uniformly distributed in a region of interest, while RL is the pattern in which, given a fixed set of points in a region, class labels are assigned to these fixed points randomly so that the labels are independent of the locations.

As alternatives, we consider two major types of spatial patterns: *segregation* and *association*. *Segregation* occurs if the NN of an individual is more likely to be of the same class as the individual than to be from a different class (see, e.g., Pielou (1961)). *Association* occurs if the NN of an individual is more likely to be from another class than to be of the same class as the individual. These patterns are not symmetric, e.g., for two classes, one class might be more associated with another class. For example, plant species  $X$  could be more dependent on species  $Y$ , so occurs in close vicinity of  $Y$  plants, while the reverse relation may not be in the same level or type. Also, class  $X$  points might exhibit a stronger clustering, compared to class  $Y$  points, and so might be more segregated compared to class  $Y$  points. See Ceyhan (2010) for more detail on the null and alternative patterns.

NNCTs are constructed using the NN frequencies of classes. The construction of NNCTs for two classes is described, e.g., in Ceyhan (2008), here we provide a brief description for  $q \geq 2$  classes. Suppose there are  $q$  classes labeled as  $\{1, 2, \dots, q\}$ . NNCTs are constructed using NN frequencies for each class. Let  $N_i$  be the number of points from class  $i$  for  $i \in \{1, 2, \dots, q\}$  and  $n = \sum_{i=1}^q N_i$ . If we record the class of each point and its nearest neighbor, the NN relationships fall into  $q^2$  categories:

$$(1, 1), (1, 2), \dots, (1, q); (2, 1), (2, 2), \dots, (2, q); \dots, (q, q)$$

where in category  $(i, j)$ , class  $i$  is the base class, while class  $j$  is the class of the NN. Denoting  $N_{ij}$  as the observed frequency of category  $(i, j)$  for  $i, j \in \{1, 2, \dots, q\}$ , we obtain the NNCT in Table 1 where  $C_j$  is

		NN class			total
		class 1	...	class $q$	
base class	class 1	$N_{11}$	...	$N_{1q}$	$n_1$
	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
	class $q$	$N_{q1}$	...	$N_{qq}$	$n_q$
total		$C_1$	...	$C_q$	$n$

Table 1: The NNCT for  $q$  classes.

the sum of column  $j$ ; i.e., number of times class  $j$  points serve as NNs for  $j \in \{1, 2, \dots, q\}$ . Note also that  $n = \sum_{i,j} N_{ij}$ ,  $n_i = \sum_{j=1}^q N_{ij}$ , and  $C_j = \sum_{i=1}^q N_{ij}$ . In cell  $(i, j)$ , class  $i$  is called the *base class*, and class  $j$  is called the *NN class*. Here we adopt the convention that variables denoted by upper case letters are random quantities, while variables denoted by lower case letters fixed quantities. Thus, in NNCT-analysis, row sums are assumed to be fixed (i.e., class sizes are given), while column sums are assumed to be random and depend on the NN relationship between the classes.

Under CSR independence or RL, cell counts  $N_{ij}$  would be close to their expected values, while under segregation the diagonal counts  $N_{ii}$  would be larger, while under association the off-diagonal counts  $N_{ij}$  would be larger than expected. When Pielou (1961) developed NNCT-tests, she used Pearson's  $\chi^2$  test of independence for testing segregation which is not appropriate due to the dependence structure in a NNCT. Dixon (1994) derived the correct asymptotic distribution of cell counts and hence the appropriate test which also has a  $\chi^2$ -distribution asymptotically. Ceyhan (2008) determines the conditions when Pielou's test is appropriate, and when Dixon's test is appropriate, and discusses their use in practice.

## 2.1 Total, Strong, and Partial Segregation and Association

When  $H_o$  is rejected, if the diagonal entries ( $N_{ii}$  values) tend to be higher than expected, there is (positive) *segregation*; if the off-diagonal entries are larger than expected, there is *association*. These types of patterns are easy to detect for  $q = 2$  classes, but for  $q > 2$ , rejecting  $H_o$  only indicates that there is some sort of deviation from the null case, but with many possible directions, since rejecting  $H_o$  only implies that for some class  $i$ , there exists classes that are more likely to serve as NN to class  $i$  or less likely to serve as NN to class  $i$  than expected under  $H_o$ . Let  $\pi_{ij}$  be the probability of a point from class  $j$  serving as NN to a point from class  $i$  given that the NN points is from class  $j$  (i.e., it is a conditional probability). For example, for a fixed class  $i$ , if  $\pi_{ii} > \sum_{j \neq i} \pi_{ij}$ , then we have *total segregation* of class  $i$  from other classes; that is, class  $i$  is more likely to have a same class NN than all other classes combined. If  $\pi_{ii} > \pi_{ij}$  for all  $i \neq j$ , then we have *strong segregation*, which implies that class  $i$  is more likely to have a con-specific NN compared to all other classes one at a time. Notice that total segregation implies strong segregation.

For fixed classes  $i$  and  $j$ , if  $\pi_{ij} > \sum_{k \neq j} \pi_{ik}$  then we have *total association* of class  $j$  with class  $i$ ; that is, class  $j$  is more likely to be a NN of class  $i$  than all other classes combined. If  $\pi_{ij} > \pi_{ik}$  for all  $k \neq j$ , then we have *strong association* of class  $j$  with class  $i$ , which implies that class  $j$  is more likely to be a NN of class  $i$  compared to all other classes one at a time. Notice that total association implies strong association.

On the other hand, if  $\pi_{ii} > \pi_{ij}$  for all  $j \in S_1 \subsetneq \{1, 2, \dots, q\} \setminus \{i\}$  and  $\pi_{ii} < \pi_{ij}$  for all  $j \in S_2 = \{1, 2, \dots, q\} \setminus (S_1 \cup \{i\})$ , then we say class  $i$  is *more segregated* from the classes in  $S_1$  and *more associated* with the classes in  $S_2$ . Such cases are called *partial segregation* of class  $i$  with respect to classes in  $S_1$  and *partial association* of class  $i$  with classes in  $S_2$ .

## 3 Cell-Specific Segregation Tests

We describe cell-specific segregation tests of Dixon and introduce new cell-specific tests labeled as type I-IV cell-specific tests, henceforth.

### 3.1 Dixon's Cell-Specific Segregation Tests

Dixon's cell-specific tests are used to measure the deviation of observed count in cell  $(i, j)$  in a NNCT from its expected value under  $H_o$  described in detail in, e.g., Dixon (1994, 2002). The test statistic suggested by Dixon for cell  $(i, j)$  is given by

$$Z_{ij}^D = \frac{N_{ij} - \mathbf{E}[N_{ij}]}{\sqrt{\mathbf{Var}[N_{ij}]}} \quad (1)$$

where  $\mathbf{E}[N_{ij}]$  is the expected cell count and  $\mathbf{Var}[N_{ij}]$  is the variance of cell count  $N_{ij}$ .

For  $q \geq 2$  classes, under RL or CSR independence, the expected cell count for cell  $(i, j)$  is

$$\mathbf{E}[N_{ij}] = \begin{cases} n_i(n_i - 1)/(n - 1) & \text{if } i = j, \\ n_i n_j/(n - 1) & \text{if } i \neq j, \end{cases} \quad (2)$$

where  $n_i$  is the fixed sample size for class  $i$  for  $i = 1, 2, \dots, q$ . Observe that the expected cell counts depend only on the size of each class (i.e., row sums), but not on column sums. And the variance is

$$\mathbf{Var}[N_{ij}] = \begin{cases} (n + R)p_{ii} + (2n - 2R + Q)p_{iii} + (n^2 - 3n - Q + R)p_{iiii} - (np_{ii})^2 & \text{if } i = j, \\ np_{ij} + Qp_{iij} + (n^2 - 3n - Q + R)p_{iijj} - (np_{ij})^2 & \text{if } i \neq j, \end{cases} \quad (3)$$

with  $p_{xx}$ ,  $p_{xxx}$ , and  $p_{xxxx}$  are the probabilities that a randomly picked pair, triplet, or quartet of points, respectively, are the indicated classes and are given by

$$\begin{aligned} p_{ii} &= \frac{n_i(n_i - 1)}{n(n - 1)}, & p_{ij} &= \frac{n_i n_j}{n(n - 1)}, \\ p_{iii} &= \frac{n_i(n_i - 1)(n_i - 2)}{n(n - 1)(n - 2)}, & p_{iij} &= \frac{n_i(n_i - 1)n_j}{n(n - 1)(n - 2)}, \\ p_{iiii} &= \frac{n_i(n_i - 1)(n_i - 2)(n_i - 3)}{n(n - 1)(n - 2)(n - 3)}, & p_{iijj} &= \frac{n_i(n_i - 1)n_j(n_j - 1)}{n(n - 1)(n - 2)(n - 3)}. \end{aligned} \quad (4)$$

Furthermore,  $R$  is twice the number of reflexive pairs and  $Q$  is the number of points with shared NNs, which occurs when two or more points share a NN. Then  $Q = 2(Q_2 + 3Q_3 + 6Q_4 + 10Q_5 + 15Q_6)$  where  $Q_k$  is the number of points that serve as a NN to other points  $k$  times.

### 3.2 Type I Cell-Specific Segregation Tests

In standard cases like multinomial sampling for contingency tables with fixed row totals and conditioning on the column totals,  $C_j = c_j$ , the expected cell count for cell  $(i, j)$  in contingency tables is  $\mathbf{E}[N_{ij}] = \frac{n_i c_j}{n}$ . We first consider the difference  $N_{ij} - \frac{n_i c_j}{n}$  for cell  $(i, j)$ . However under RL,  $N_i = n_i$  are fixed, but  $C_j$  are random quantities and  $C_j = \sum_{i=1}^q N_{ij}$ , hence we suggest as the first type of cell-specific segregation test as

$$T_{ij}^I = N_{ij} - \frac{n_i C_j}{n}.$$

Then under RL,

$$\mathbf{E}[T_{ij}^I] = \begin{cases} \frac{n_i(n_i - 1)}{(n - 1)} - \frac{n_i}{n} \mathbf{E}[C_i] & \text{if } i = j, \\ \frac{n_i n_j}{(n - 1)} - \frac{n_i}{n} \mathbf{E}[C_j] & \text{if } i \neq j. \end{cases} \quad (5)$$

For all  $j$ ,  $\mathbf{E}[C_j] = n_j$ , since

$$\begin{aligned} \mathbf{E}[C_j] &= \sum_{i=1}^q \mathbf{E}[N_{ij}] = \frac{n_j(n_j - 1)}{(n - 1)} + \sum_{i \neq j} \frac{n_i n_j}{(n - 1)} = \frac{n_j(n_j - 1)}{(n - 1)} + \frac{n_j}{(n - 1)} \sum_{i \neq j} n_i \\ &= \frac{n_j(n_j - 1)}{(n - 1)} + \frac{n_j}{(n - 1)}(n - n_j) = n_j. \end{aligned}$$

Therefore,

$$\mathbf{E} [T_{ij}^I] = \begin{cases} \frac{n_i(n_i-1)}{n(n-1)} & \text{if } i = j, \\ \frac{n_i n_j}{n(n-1)} & \text{if } i \neq j. \end{cases} \quad (6)$$

For the variance of  $T_{ij}^I$ , we have

$$\mathbf{Var} [T_{ij}^I] = \mathbf{Var}[N_{ij}] + \frac{n_i^2}{n^2} \mathbf{Var}[C_j] - 2 \frac{n_i}{n} \mathbf{Cov}[N_{ij}, C_j] \quad (7)$$

where  $\mathbf{Var}[N_{ij}]$  are as in Equation (3),  $\mathbf{Var}[C_j] = \sum_{i=1}^q \mathbf{Var}[N_{ij}] + \sum_{k \neq i} \sum_i \mathbf{Cov}[N_{ij}, N_{kj}]$  and  $\mathbf{Cov}[N_{ij}, C_j] = \sum_{k=1}^q \mathbf{Cov}[N_{ij}, N_{kj}]$  with  $\mathbf{Cov}[N_{ij}, N_{kl}]$  are as in Equations (4)-(12) of Dixon (2002).

As a new cell-specific test, we propose

$$Z_{ij}^I = \frac{T_{ij}^I - \mathbf{E} [T_{ij}^I]}{\sqrt{\mathbf{Var} [T_{ij}^I]}}. \quad (8)$$

### 3.3 Type II Cell-Specific Segregation Tests

In Section 3.2, we suggested  $N_{ij} - \frac{n_i C_j}{n}$  as the test statistic for cell  $(i, j)$ . However, under RL,  $\mathbf{E}[C_j] = n_j$ , so we suggest as the second type of segregation test as

$$T_{ij}^{II} = N_{ij} - \frac{n_i n_j}{n}.$$

Then under RL,  $\mathbf{E} [T_{ij}^{II}] = \mathbf{E} [T_{ij}^I]$  which is provided in Equation (6). Moreover, the variance of  $T_{ij}^I$  is  $\mathbf{Var} [T_{ij}^{II}] = \mathbf{Var}[N_{ij}]$ , since  $n_i$ ,  $n_j$  and  $n$  are fixed.

As a cell-specific test, we propose

$$Z_{ij}^{II} = \frac{T_{ij}^{II} - \mathbf{E} [T_{ij}^{II}]}{\sqrt{\mathbf{Var} [T_{ij}^{II}]}}, \quad (9)$$

### 3.4 Type III Cell-Specific Segregation Tests

In the previous sections,  $\mathbf{E} [T_{ij}^I] = \mathbf{E} [T_{ij}^{II}] \neq 0$  under RL. Hence, instead of these test statistics, in order to obtain 0 expected value for our test statistic, we suggest the following:

$$T_{ij}^{III} = \begin{cases} N_{ii} - \frac{(n_i-1)}{(n-1)} C_i & \text{if } i = j, \\ N_{ij} - \frac{n_i}{(n-1)} C_j & \text{if } i \neq j. \end{cases} \quad (10)$$

Then  $\mathbf{E} [T_{ij}^{III}] = 0$ , since, for  $i = j$ ,

$$\mathbf{E} [T_{ii}^{III}] = \mathbf{E}[N_{ii}] - \frac{(n_i-1)}{(n-1)} \mathbf{E}[C_i] = \frac{n_i(n_i-1)}{(n-1)} - \frac{(n_i-1)}{(n-1)} n_i = 0,$$

and for  $i \neq j$ ,

$$\mathbf{E} [T_{ij}^{III}] = \mathbf{E}[N_{ij}] - \frac{(n_i-1)}{(n-1)} \mathbf{E}[C_j] = \frac{n_i n_j}{(n-1)} - \frac{(n_i-1)}{(n-1)} n_j = 0.$$

As for the variance of  $T_{ij}^{III}$ , we have

$$\mathbf{Var} [T_{ij}^{III}] = \begin{cases} \mathbf{Var}[N_{ij}] + \frac{(n_i-1)^2}{(n-1)^2} \mathbf{Var}[C_j] - 2 \frac{(n_i-1)}{(n-1)} \mathbf{Cov}[N_{ij}, C_j] & \text{if } i = j, \\ \mathbf{Var}[N_{ij}] + \frac{n_i^2}{(n-1)^2} \mathbf{Var}[C_j] - 2 \frac{n_i}{(n-1)} \mathbf{Cov}[N_{ij}, C_j] & \text{if } i \neq j. \end{cases} \quad (11)$$

As a new cell-specific test, we propose

$$Z_{ij}^{III} = \frac{T_{ij}^{III}}{\sqrt{\mathbf{Var}[T_{ij}^{III}]}}. \quad (12)$$

Notice that this is same as the new cell-specific test introduced in (Ceyhan (2010)), and details of this test are provided for the sake of completeness.

### 3.5 Type IV Cell-Specific Segregation Tests

For  $T_{ij}^{III}$ , we introduced a coefficient in front of the second term, i.e.,  $n_i C_j/n$ , to obtain a zero expected value for our statistic under RL. In this section, we modify the first term and obtain the following test statistic:

$$T_{ij}^{IV} = \begin{cases} \frac{n_i(n-1)}{n(n_i-1)}N_{ij} - \frac{n_i}{n}C_j = \frac{n_i}{n} \left( \frac{n-1}{n_i-1}N_{ij} - C_j \right) & \text{if } i = j, \\ \frac{n-1}{n}N_{ij} - \frac{n_i}{n}C_j = \frac{1}{n}((n-1)N_{ij} - n_i C_j) & \text{if } i \neq j. \end{cases} \quad (13)$$

Then  $\mathbf{E}[T_{ij}^{IV}] = 0$ , since, for  $i = j$ ,

$$\mathbf{E}[T_{ii}^{IV}] = \frac{n_i}{n} \left( \frac{n-1}{n_i-1} \mathbf{E}[N_{ii}] - \mathbf{E}[C_i] \right) = \frac{n_i}{n} \left( \frac{n-1}{n_i-1} \frac{n_i(n_i-1)}{n-1} - n_i \right) = 0,$$

and for  $i \neq j$ ,

$$\mathbf{E}[T_{ij}^{IV}] = \frac{1}{n}((n-1)\mathbf{E}[N_{ij}] - n_i \mathbf{E}[C_j]) = \frac{1}{n} \left( (n-1) \frac{n_i n_j}{n-1} - n_i n_j \right) = 0.$$

As for the variance of  $T_{ij}^{IV}$ , we have

$$\mathbf{Var}[T_{ij}^{IV}] = \begin{cases} \frac{n_i^2}{n^2} \left( \frac{(n-1)^2}{(n_i-1)^2} \mathbf{Var}[N_{ii}] + \mathbf{Var}[C_i] - 2 \frac{(n-1)}{(n_i-1)} \mathbf{Cov}[N_{ii}, C_i] \right) & \text{if } i = j, \\ \frac{1}{n^2} ((n-1)^2 \mathbf{Var}[N_{ij}] + n_i^2 \mathbf{Var}[C_j] - 2(n-1)n_i \mathbf{Cov}[N_{ij}, C_j]) & \text{if } i \neq j. \end{cases} \quad (14)$$

As a new cell-specific test, we propose

$$Z_{ij}^{IV} = \frac{T_{ij}^{IV}}{\sqrt{\mathbf{Var}[T_{ij}^{IV}]}}. \quad (15)$$

## 4 Overall Segregation Tests

In this section, we describe the overall segregation tests in literature and introduce new overall tests based on cell-specific tests in Section 3.

### 4.1 Dixon's Overall Segregation Test

In the multi-class case with  $q$  classes, combining the  $q^2$  cell-specific tests in Section 3.1, Dixon (2002) suggests the quadratic form to obtain the overall segregation test as follows:

$$C_D = (\mathbf{N} - \mathbf{E}[\mathbf{N}])' \Sigma_D^- (\mathbf{N} - \mathbf{E}[\mathbf{N}]) \quad (16)$$

where  $\mathbf{N}$  is the  $q^2 \times 1$  vector of  $q$  rows of the NNCT concatenated row-wise,  $\mathbf{E}[\mathbf{N}]$  is the vector of  $\mathbf{E}[N_{ij}]$  which are as in Equation (2),  $\Sigma_D$  is the  $q^2 \times q^2$  variance-covariance matrix for the cell count vector  $\mathbf{N}$  with diagonal entries equal to  $\mathbf{Var}[N_{ij}]$  and off-diagonal entries being  $\mathbf{Cov}[N_{ij}, N_{kl}]$  for  $(i, j) \neq (k, l)$ . The explicit forms of the variance and covariance terms are provided in (Dixon (2002)). Also,  $\Sigma_D^-$  is a generalized inverse of  $\Sigma_D$  (Searle (2006)) and  $'$  stands for the transpose of a vector or matrix. Then under RL,  $C_D$  has a  $\chi_{q(q-1)}^2$  distribution asymptotically.

## 4.2 Type I Overall Segregation Test

We can also combine the type I cell-specific tests of Section 3.2. Let  $\mathbf{T}^I$  be the vector of  $q^2 T_{ij}^I$  values, i.e.,

$$\mathbf{T}^I = (T_{11}^I, T_{12}^I, \dots, T_{1q}^I, T_{21}^I, T_{22}^I, \dots, T_{2q}^I, \dots, T_{qq}^I)',$$

and let  $\mathbf{E}[\mathbf{T}^I]$  be the vector of  $\mathbf{E}[T_{ij}^I]$  values. Note that  $\mathbf{E}[\mathbf{T}^I] = (\mathbf{E}[T_{11}^I], \mathbf{E}[T_{12}^I], \dots, \mathbf{E}[T_{1q}^I], \mathbf{E}[T_{21}^I], \mathbf{E}[T_{22}^I], \dots, \mathbf{E}[T_{2q}^I], \dots, \mathbf{E}[T_{qq}^I])'$ . Hence to obtain a new overall segregation test, referred to as type I overall test, we use the following quadratic form:

$$C_I = (\mathbf{T}^I - \mathbf{E}[\mathbf{T}^I])' \Sigma_I^{-1} (\mathbf{T}^I - \mathbf{E}[\mathbf{T}^I]) \quad (17)$$

where  $\Sigma_I$  is the  $q^2 \times q^2$  variance-covariance matrix of  $\mathbf{T}^I$ .

Under RL, the diagonal entries in the variance-covariance matrix  $\Sigma_I$  are  $\mathbf{Var}[T_{ij}^I]$  which are provided in Equation (7). For the off-diagonal entries in  $\Sigma_I$ , i.e.,  $\mathbf{Cov}[T_{ij}^I, T_{kl}^I]$  with  $(i, j) \neq (k, l)$ , there are four cases to consider:

**case 1:**  $i = j$  and  $k = l$ , then

$$\begin{aligned} \mathbf{Cov}[T_{ii}^I, T_{kk}^I] &= \mathbf{Cov}\left[N_{ii} - \frac{n_i}{n}C_i, N_{kk} - \frac{n_k}{n}C_k\right] = \\ &\mathbf{Cov}[N_{ii}, N_{kk}] - \frac{n_k}{n}\mathbf{Cov}[N_{ii}, C_k] - \frac{n_i}{n}\mathbf{Cov}[N_{kk}, C_i] + \frac{n_i n_k}{n^2}\mathbf{Cov}[C_i, C_k]. \end{aligned} \quad (18)$$

**case 2:**  $i = j$  and  $k \neq l$ , then

$$\begin{aligned} \mathbf{Cov}[T_{ii}^I, T_{kl}^I] &= \mathbf{Cov}\left[N_{ii} - \frac{n_i}{n}C_i, N_{kl} - \frac{n_k}{n}C_l\right] = \\ &\mathbf{Cov}[N_{ii}, N_{kl}] - \frac{n_k}{n}\mathbf{Cov}[N_{ii}, C_l] - \frac{n_i}{n}\mathbf{Cov}[N_{kl}, C_i] + \frac{n_i n_k}{n^2}\mathbf{Cov}[C_i, C_l]. \end{aligned} \quad (19)$$

**case 3:**  $i \neq j$  and  $k = l$ , then  $\mathbf{Cov}[T_{ij}^I, T_{kk}^I] = \mathbf{Cov}[T_{kk}^I, T_{ij}^I]$ , which is essentially **case 2** above.

**case 4:**  $i \neq j$  and  $k \neq l$ , then

$$\begin{aligned} \mathbf{Cov}[T_{ij}^I, T_{kl}^I] &= \mathbf{Cov}\left[N_{ij} - \frac{n_i}{n}C_j, N_{kl} - \frac{n_k}{n}C_l\right] = \\ &\mathbf{Cov}[N_{ij}, N_{kl}] - \frac{n_k}{n}\mathbf{Cov}[N_{ij}, C_l] - \frac{n_i}{n}\mathbf{Cov}[N_{kl}, C_j] + \frac{n_i n_k}{n^2}\mathbf{Cov}[C_j, C_l]. \end{aligned} \quad (20)$$

## 4.3 Type II Overall Segregation Test

We also combine the type II cell-specific tests of Section 3.3. Let  $\mathbf{T}^{II}$  be the vector of  $q^2 T_{ij}^{II}$  values, i.e.,

$$\mathbf{T}^{II} = (T_{11}^{II}, T_{12}^{II}, \dots, T_{1q}^{II}, T_{21}^{II}, T_{22}^{II}, \dots, T_{2q}^{II}, \dots, T_{qq}^{II})',$$

and let  $\mathbf{E}[\mathbf{T}^{II}]$  be the vector of  $\mathbf{E}[T_{ij}^{II}]$  values. As the type II overall segregation test, we use the following quadratic form:

$$C_N = (\mathbf{T}^{II} - \mathbf{E}[\mathbf{T}^{II}])' \Sigma_{II}^{-1} (\mathbf{T}^{II} - \mathbf{E}[\mathbf{T}^{II}]) \quad (21)$$

where  $\Sigma_{II}$  is the  $q^2 \times q^2$  variance-covariance matrix of  $\mathbf{T}^{II}$ .

Under RL, the diagonal entries in the variance-covariance matrix  $\Sigma_N$  are  $\mathbf{Var}[T_{ij}^{II}]$  which are same as  $\mathbf{Var}[N_{ij}]$ . For the off-diagonal entries in  $\Sigma_{II}$ , i.e.,  $\mathbf{Cov}[T_{ij}^{II}, T_{kl}^{II}]$  with  $(i, j) \neq (k, l)$ , we have  $\mathbf{Cov}[T_{ij}^{II}, T_{kl}^{II}] = \mathbf{Cov}[N_{ij} - \frac{n_i n_j}{n}, N_{kl} - \frac{n_k n_l}{n}] = \mathbf{Cov}[N_{ij}, N_{kl}]$ .

#### 4.4 Type III Overall Segregation Test

When we combine the type III cell-specific tests of Section 3.4, we obtain type III overall test as follows. Let  $\mathbf{T}^{III}$  be the vector of  $q^2$   $T_{ij}^{III}$  values, i.e.,

$$\mathbf{T}^{III} = (T_{11}^{III}, T_{12}^{III}, \dots, T_{1q}^{III}, T_{21}^{III}, T_{22}^{III}, \dots, T_{2q}^{III}, \dots, T_{qq}^{III})',$$

and let  $\mathbf{E}[\mathbf{T}^{III}]$  be the vector of  $\mathbf{E}[T_{ij}^{III}]$  values. Note that  $\mathbf{E}[\mathbf{T}^{III}] = \mathbf{0}$ . As the type III overall segregation test, we use the following quadratic form:

$$C_{III} = (\mathbf{T}^{III})' \Sigma_{III}^{-} (\mathbf{T}^{III}) \quad (22)$$

where  $\Sigma_{III}$  is the  $q^2 \times q^2$  variance-covariance matrix of  $\mathbf{T}^{III}$ .

Under RL, the diagonal entries in the variance-covariance matrix  $\Sigma_{III}$  are  $\mathbf{Var}[T_{ij}^{III}]$  which are provided in Equation (11). For the off-diagonal entries in  $\Sigma_{III}$ , i.e.,  $\mathbf{Cov}[T_{ij}^{III}, T_{kl}^{III}]$  with  $(i, j) \neq (k, l)$ , there are four cases to consider:

**case 1:**  $i = j$  and  $k = l$ , then

$$\begin{aligned} \mathbf{Cov}[T_{ii}^{III}, T_{kk}^{III}] &= \mathbf{Cov}\left[N_{ii} - \frac{(n_i - 1)}{(n - 1)}C_i, N_{kk} - \frac{(n_k - 1)}{(n - 1)}C_k\right] = \\ &\mathbf{Cov}[N_{ii}, N_{kk}] - \frac{(n_k - 1)}{(n - 1)}\mathbf{Cov}[N_{ii}, C_k] - \frac{(n_i - 1)}{(n - 1)}\mathbf{Cov}[N_{kk}, C_i] + \frac{(n_i - 1)(n_k - 1)}{(n - 1)^2}\mathbf{Cov}[C_i, C_k]. \end{aligned} \quad (23)$$

**case 2:**  $i = j$  and  $k \neq l$ , then

$$\begin{aligned} \mathbf{Cov}[T_{ii}^{III}, T_{kl}^{III}] &= \mathbf{Cov}\left[N_{ii} - \frac{(n_i - 1)}{(n - 1)}C_i, N_{kl} - \frac{n_k}{(n - 1)}C_l\right] = \\ &\mathbf{Cov}[N_{ii}, N_{kl}] - \frac{n_k}{(n - 1)}\mathbf{Cov}[N_{ii}, C_l] - \frac{(n_i - 1)}{(n - 1)}\mathbf{Cov}[N_{kl}, C_i] + \frac{(n_i - 1)n_k}{(n - 1)^2}\mathbf{Cov}[C_i, C_l]. \end{aligned} \quad (24)$$

**case 3:**  $i \neq j$  and  $k = l$ , then  $\mathbf{Cov}[T_{ij}^{III}, T_{kk}^{III}] = \mathbf{Cov}[T_{kk}^{III}, T_{ij}^{III}]$ , which is essentially **case 2** above.

**case 4:**  $i \neq j$  and  $k \neq l$ , then

$$\begin{aligned} \mathbf{Cov}[T_{ij}^{III}, T_{kl}^{III}] &= \mathbf{Cov}\left[N_{ij} - \frac{n_i}{(n - 1)}C_j, N_{kl} - \frac{n_k}{(n - 1)}C_l\right] = \\ &\mathbf{Cov}[N_{ij}, N_{kl}] - \frac{n_k}{(n - 1)}\mathbf{Cov}[N_{ij}, C_l] - \frac{n_i}{(n - 1)}\mathbf{Cov}[N_{kl}, C_j] + \frac{n_i n_k}{(n - 1)^2}\mathbf{Cov}[C_j, C_l]. \end{aligned} \quad (25)$$

Note that type III overall segregation is same as the new overall test provided in (Ceyhan (2010)).

#### 4.5 Type IV Overall Segregation Test

When we combine the type IV cell-specific tests of Section 3.5, we obtain type IV overall test as follows. Let  $\mathbf{T}^{IV}$  be the vector of  $q^2$   $T_{ij}^{IV}$  values, i.e.,

$$\mathbf{T}^{IV} = [T_{11}^{IV}, T_{12}^{IV}, \dots, T_{1q}^{IV}, T_{21}^{IV}, T_{22}^{IV}, \dots, T_{2q}^{IV}, \dots, T_{qq}^{IV}]',$$

and let  $\mathbf{E}[\mathbf{T}^{IV}]$  be the vector of  $\mathbf{E}[T_{ij}^{IV}]$  values. Note that  $\mathbf{E}[\mathbf{T}^{IV}] = \mathbf{0}$ . As the type IV overall segregation test, we use the following quadratic form:

$$C_{IV} = (\mathbf{T}^{IV})' \Sigma_{IV}^{-} (\mathbf{T}^{IV}) \quad (26)$$

where  $\Sigma_{IV}$  is the  $q^2 \times q^2$  variance-covariance matrix of  $\mathbf{T}^{IV}$ .



Under RL, the diagonal entries in the variance-covariance matrix  $\Sigma_{IV}$  are  $\mathbf{Var}[T_{ij}^{IV}]$  which are provided in Equation (14). For the off-diagonal entries in  $\Sigma_{IV}$ , i.e.,  $\mathbf{Cov}[T_{ij}^{IV}, T_{kl}^{IV}]$  with  $(i, j) \neq (k, l)$ , there are four cases to consider:

**case 1:**  $i = j$  and  $k = l$ , then

$$\begin{aligned} \mathbf{Cov}[T_{ii}^{IV}, T_{kk}^{IV}] &= \mathbf{Cov}\left[\frac{n_i}{n}\left(\frac{n-1}{n_i-1}N_{ii} - C_i\right), \frac{n_k}{n}\left(\frac{n-1}{n_k-1}N_{kk} - \frac{(n_k-1)}{(n-1)}C_k\right)\right] = \\ &= \frac{n_i n_k}{n^2} \mathbf{Cov}\left[\frac{n-1}{n_i-1}N_{ii} - C_i, \frac{n-1}{n_k-1}N_{kk} - \frac{(n_k-1)}{(n-1)}C_k\right] = \\ &= \frac{n_i n_k}{n^2} \left( \frac{(n-1)^2}{(n_i-1)(n_k-1)} \mathbf{Cov}[N_{ii}, N_{kk}] - \frac{(n-1)}{(n_i-1)} \mathbf{Cov}[N_{ii}, C_k] - \frac{(n-1)}{(n_k-1)} \mathbf{Cov}[N_{kk}, C_i] + \mathbf{Cov}[C_i, C_k] \right). \end{aligned} \quad (27)$$

**case 2:**  $i = j$  and  $k \neq l$ , then

$$\begin{aligned} \mathbf{Cov}[T_{ii}^{IV}, T_{kl}^{IV}] &= \mathbf{Cov}\left[\frac{n_i}{n}\left(\frac{n-1}{n_i-1}N_{ii} - C_i\right), \frac{1}{n}((n-1)N_{kl} - n_k C_l)\right] = \\ &= \frac{n_i}{n^2} \mathbf{Cov}\left[\frac{n-1}{n_i-1}N_{ii} - C_i, (n-1)N_{kl} - n_k C_l\right] = \\ &= \frac{n_i}{n^2} \left( \frac{(n-1)^2}{(n_i-1)(n_k-1)} \mathbf{Cov}[N_{ii}, N_{kl}] - \frac{(n-1)n_k}{(n_i-1)} \mathbf{Cov}[N_{ii}, C_l] - (n-1) \mathbf{Cov}[N_{kl}, C_i] + n_k \mathbf{Cov}[C_i, C_l] \right). \end{aligned} \quad (28)$$

**case 3:**  $i \neq j$  and  $k = l$ , then  $\mathbf{Cov}[T_{ij}^{IV}, T_{kk}^{IV}] = \mathbf{Cov}[T_{kk}^{IV}, T_{ij}^{IV}]$ , which is essentially **case 2** above.

**case 4:**  $i \neq j$  and  $k \neq l$ , then

$$\begin{aligned} \mathbf{Cov}[T_{ij}^{IV}, T_{kl}^{IV}] &= \mathbf{Cov}\left[\frac{1}{n}((n-1)N_{ij} - n_i C_j), \frac{1}{n}((n-1)N_{kl} - n_k C_l)\right] = \\ &= \frac{1}{n^2} \mathbf{Cov}[(n-1)N_{ij} - n_i C_j, (n-1)N_{kl} - n_k C_l] = \\ &= \frac{1}{n^2} \left( (n-1)^2 \mathbf{Cov}[N_{ij}, N_{kl}] - (n-1)n_k \mathbf{Cov}[N_{ij}, C_l] - (n-1)n_i \mathbf{Cov}[N_{kl}, C_j] + n_i n_k \mathbf{Cov}[C_j, C_l] \right). \end{aligned} \quad (29)$$

## 4.6 Remarks on NNCT-Tests

Under RL,  $Z_{ii}^D$  is shown to have  $N(0, 1)$  distribution asymptotically, while for  $q > 2$  the asymptotic normality of the off-diagonal cells in NNCTs is not rigorously established, although extensive Monte Carlo simulations indicate approximate normality for large samples (Dixon (2002)). Furthermore, Dixon's cell specific test and type II cell-specific test are equivalent, and so are types III and IV cell-specific tests.

Asymptotically, under RL  $C_D$  and  $C_{II}$  has a  $\chi_{q(q-1)}^2$  distribution since rank of  $\Sigma_D$  and  $\Sigma_{II}$  is  $q(q-1)$ , in fact,  $\Sigma_D = \Sigma_{II}$ .  $C_{III}$  has a  $\chi_{(q-1)^2}^2$  distribution since rank of  $\Sigma_{III}$  is  $(q-1)^2$ . However, our Monte Carlo simulations suggest that  $C_I$  has  $\chi_\nu^2$  distribution where  $\nu = (q-1)^2 - 1/2$ , while  $C_{IV}$  has  $\chi_\nu^2$  distribution where  $\nu = q^2 - 2$ . Furthermore, the cell-specific test statistics are dependent, hence their squares do not sum to the corresponding overall segregation tests. Among the overall tests, Dixon's test and type II overall test are identical (the small differences in practice are due to rounding errors in computations).

In all the above cases,  $\mathbf{Cov}[N_{ij}, N_{kl}]$  are as in Dixon (2002),  $\mathbf{Cov}[N_{ij}, C_l] = \sum_{k=1}^q \mathbf{Cov}[N_{ij}, N_{kl}]$  and  $\mathbf{Cov}[C_i, C_j] = \sum_{k=1}^q \sum_{l=1}^q \mathbf{Cov}[N_{ki}, N_{lj}]$ .

Under CSR independence, the cell-specific and overall tests are as in RL case. However, under RL,  $Q$  and  $R$  are fixed quantities, as they depend only on the location of the points, but not the types of NNs, while under CSR independence, they are random. Under CSR independence, the distribution of the test statistics above is similar to the RL case. The only difference is that the new cell-specific tests asymptotically have

$N(0,1)$  distribution conditional on  $Q$  and  $R$ . Hence, under CSR independence,  $\mathbf{Var}[N_{ij}]$ ,  $\mathbf{Cov}[N_{ij}, N_{kl}]$ ,  $\mathbf{Cov}[N_{ij}, C_k]$ ,  $\mathbf{Cov}[C_i, C_j]$ , and all other quantities depending on  $Q$  and  $R$  are conditional on  $Q$  and  $R$ . The unconditional variances can be obtained by replacing  $Q$  and  $R$  with their expectations (see Ceyhan (2010) for more detail). Since  $Q$  and  $R$  are random under CSR independence, the variances of the test statistics tend to be larger compared to the ones under RL.

Each of the cell-specific tests measures the deviation of the test statistic from its expected value under  $H_0$ . Dixon's and type II cell-specific tests depend on  $N_{ij}$  (i.e., cell counts) and row sums only, and types I, III, and IV cell-specific tests incorporate column sums as well. For the cell-specific tests, the  $z$ -score for cell  $(i, j)$  indicates the level and direction of spatial interaction between classes  $i$  and  $j$ . If the  $z$ -score for cell  $(i, i)$  is significantly larger (less) than zero, then class  $i$  exhibits (lack of) segregation from other classes. If the  $z$ -score for cell  $(i, j)$  with  $i \neq j$  is significantly larger (less) than zero, then class  $j$  exhibits (lack of) association with class  $i$ . Moreover, for cells  $(i, j)$  with  $i \neq j$ , the cell-specific tests are not symmetric. For example, the cell-specific test for cell  $(i, j)$  may exhibit a different level of interaction compared to the cell  $(j, i)$ . The overall tests combine cell-specific tests in one compound summary statistic. The performance of cell-specific tests are expected to carry over to the overall tests, provided the correct degrees of freedom is determined.

Recall that in the two-class case, each cell count  $N_{ij}$  has asymptotic normal distribution (Cuzick and Edwards (1990)). Hence, the new cell-specific tests  $Z_{ij}^I$ ,  $Z_{ij}^{II}$ ,  $Z_{ij}^{III}$  and  $Z_{ij}^{IV}$  also converges in law to  $N(0,1)$  as  $n \rightarrow \infty$ . Moreover, one and two-sided versions of these tests are also possible. In the two-class case, usually only two cells contain all the information provided by the NNCT. In particular, segregation of class  $i$  from class  $j$  implies lack of association between classes  $i$  and  $j$  ( $i \neq j$ ) and lack of segregation of class  $i$  from class  $j$  implies association between classes  $i$  and  $j$  ( $i \neq j$ ). For Dixon's cell-specific test, we have  $Z_{i1}^D = -Z_{i2}^D$  for  $i = 1, 2$ . For type I cell-specific test,  $Z_{11}^I = Z_{22}^I = -Z_{12}^I = -Z_{21}^I$ ; and for type II cell-specific test, we have  $Z_{ij}^D = Z_{ij}^{II}$ ; for type III cell-specific test, we have  $Z_{1j}^{III} = -Z_{2j}^{III}$  for  $j = 1, 2$ ; and for type IV cell-specific test, we have  $Z_{ij}^{III} = Z_{ij}^{IV}$ .

In the multi-class case, a positive  $z$ -score for the diagonal cell  $(i, i)$  indicates segregation, but it does not necessarily mean lack of association between class  $i$  and class  $j$  ( $i \neq j$ ), since it could be the case that class  $i$  could be associated with one class, yet not associated with another one. See also Section 2.1.

The cell-specific and overall tests are all consistent under both segregation and association alternative, which can be shown with the same mechanism as in (Ceyhan (2008)).

## 4.7 Post-hoc Tests after Overall Tests: Class-Specific, Pairwise, and One-vs-rest Type Tests

In our construction of the NNCT-tests, although we first introduce the cell-specific tests and then develop overall tests based on the cell-specific tests, in practice it is more natural to conduct the tests in reverse order. That is, first an overall NNCT-test should be performed, and if significant, then one can perform cell-specific tests to determine the types and levels of the spatial interaction patterns between the classes. This procedure is in fact analogous to ANOVA  $F$ -test to compare multiple groups, in the sense that if the  $F$ -test yields a significant result, then one performs pairwise tests to determine which pairs are different.

However, NNCT-tests provide more alternatives (compared to ANOVA  $F$ -test) as post-hoc tests after an overall test is significant. In the multi-class case, when an overall test is rejected; i.e., there is evidence in favor of some sort of deviation from randomness of the spatial pattern, the next natural question is what type of deviation occurs for each class (or species). To this end, one can conduct several post-hoc tests. One type of post-hoc tests is the class-specific tests discussed in Dixon (2002) and Ceyhan (2009). For pairwise comparison of the interaction between classes, one can resort to two options: (i) in a  $q \times q$  NNCT, one can consider cell-specific tests for each cell (which also provides interaction of the class with itself on the diagonal cells) and (ii) one can restrict attention to the pair of classes  $i, j$  with  $i \neq j$  one at a time and conduct the tests as in the two-class case with a  $2 \times 2$  NNCT. We recommend the approach in (i), since it incorporates all the classes in question and provides the types of interaction in the presence of all classes, while the approach in (ii) ignores the possible confounding effects of classes different from the pair in question. This in practice might not give the exact picture of the mixed relationships between all the classes.

As another alternative post-hoc procedure, Dixon (2002) suggested the following. For class  $j$ , we pool the remaining classes and treat them as the other class in a two-class setting. Then we apply the two-class tests to the resulting NNCT. To emphasize the difference, this version of the class-specific test is called *one-vs-rest type test*. For  $q > 2$  classes, let  $\mathcal{N}$  be the  $q \times q$  NNCT with cell counts being  $N_{ij}$  and let  $\tilde{\mathcal{N}}$  be the  $2 \times 2$  NNCT for the one-versus-rest type procedure with cell counts being  $\tilde{N}_{ij}$ . When we are performing a one-versus-rest type testing for class  $i$ , without loss of generality, we can assign the first row in  $\tilde{\mathcal{N}}$  to class  $i$  and the second row to the rest. Then  $\tilde{N}_{11} = N_{ii}$ ,  $\tilde{N}_{12} = \sum_{j \neq i} N_{ij}$ ,  $\tilde{N}_{21} = \sum_{j \neq i} N_{ji}$ , and  $\tilde{N}_{22} = \sum_{j \neq i, k \neq i} N_{jk}$ . Hence in the one-versus-rest type testing, the cell-specific test for cell  $(1, 1)$  in  $\tilde{\mathcal{N}}$  would be same as the cell-specific test for cell  $(i, i)$  in  $\mathcal{N}$ . Therefore, to extract information from  $\tilde{\mathcal{N}}$  that is not provided by  $\mathcal{N}$ , we consider the cell-specific tests for cell  $(2, 2)$  in  $\tilde{\mathcal{N}}$ . The overall test statistics for  $\tilde{\mathcal{N}}$  are also different than the ones for  $\mathcal{N}$ .

In a multi-class case with  $q \geq 2$  classes, there are  $q$  class-specific and one-vs-rest types of tests and  $\binom{q}{2} = q(q-1)/2$  pairwise tests and  $q^2$  cell-specific tests. As  $q$  increases the class-specific tests are less intensive computationally and easier to interpret, whereas the pairwise tests might yield conflicting results.

## 5 Empirical Significance Levels in the Two-Class Case

We provide the empirical significance levels for Dixon's and the new cell-specific and overall segregation tests in the two-class case under CSR independence and RL patterns. Our Monte Carlo simulation set-up is same as in Ceyhan (2010).

### 5.1 Empirical Significance Levels under CSR Independence of Two Classes

For CSR independence pattern, in the two-class case, we label the classes as  $X$  and  $Y$ , or class 1 and class 2, interchangeably. We generate  $n_1$  points from class  $X$  and  $n_2$  points from class  $Y$  both of which are independent of each other and independently uniformly distributed on the unit square,  $(0, 1) \times (0, 1)$ . We use the sample size combinations  $(n_1, n_2) \in \{(10, 10), (10, 30), (10, 50), (30, 30), (30, 50), (50, 50), (50, 100), (100, 100)\}$  and perform  $N_{mc} = 10000$  replications. The empirical sizes are calculated as the ratio of number of significant results to the number of Monte Carlo replications,  $N_{mc}$ . We use .05 as our nominal significance level.

We present the empirical significance levels for the NNCT-tests in Figure 1. The empirical sizes significantly smaller (larger) than .05 are deemed as conservative (liberal). The asymptotic normal approximation to proportions are used in determining the significance of the deviations of the empirical sizes from the nominal level of .05. For these proportion tests, we also use  $\alpha = .05$  to test against empirical size being equal to .05. With  $N_{mc} = 10000$ , empirical sizes less than .0464 are deemed conservative, greater than .0536 are deemed liberal at  $\alpha = .05$  level. These thresholds are indicated as the horizontal lines in Figure 1. Note also that the sample sizes are arranged in the increasing order for the first and then the second entries. The size values for discrete sample size combinations are joined by piecewise straight lines for better visualization. Let  $\hat{\alpha}_{i,j}^D$ ,  $\hat{\alpha}_{i,j}^I$ - $\hat{\alpha}_{i,j}^{IV}$  are the empirical significance levels of Dixon's and the cell-specific tests of types I-IV, respectively,  $\hat{\alpha}_D$  is for Dixon's and  $\hat{\alpha}_I$ - $\hat{\alpha}_{IV}$  is for the overall segregation tests. Notice that in the two-class case  $\hat{\alpha}_{1,1}^D = \hat{\alpha}_{1,2}^D$  and  $\hat{\alpha}_{2,1}^D = \hat{\alpha}_{2,2}^D$ , since  $N_{12} = n_1 - N_{11}$  and  $N_{21} = n_2 - N_{22}$ . Likewise for  $\hat{\alpha}_{i,j}^I$ - $\hat{\alpha}_{i,j}^{IV}$ . So we only present cell-specific tests for cells  $(1, 1)$  and  $(2, 2)$ . Furthermore, since Dixon's cell specific test and type II cell-specific test are equivalent, and so are types III and IV cell-specific tests, we only present Dixon's, types I and III cell-specific tests.

For cell  $(1, 1)$ , Dixon's cell-specific test has empirical size close to the nominal level of 0.05 for balanced sample sizes (i.e., for  $n_1 \approx n_2$  or when relative abundance of classes are similar), while for unbalanced sample sizes, it tends to be liberal or conservative. On the other hand, types I and III cell-specific tests are less severely affected by the differences in relative abundances of the classes, i.e., they are closer to the nominal level for all sample size combinations. For cell  $(2, 2)$ , Dixon's cell-specific test is much closer to 0.05 for all sample size combinations, while types I and III cell-specific tests have similar performance as in cell  $(1, 1)$ . Thus, Dixon's cell-specific test has much better empirical size performance for the diagonal cell corresponding to the class with larger size, while types I and III cell-specific tests have better size performance for the diagonal cell corresponding to the class with smaller size.

## Empirical Size Plots for the NNCT-Tests under CSR Independence of Two Classes

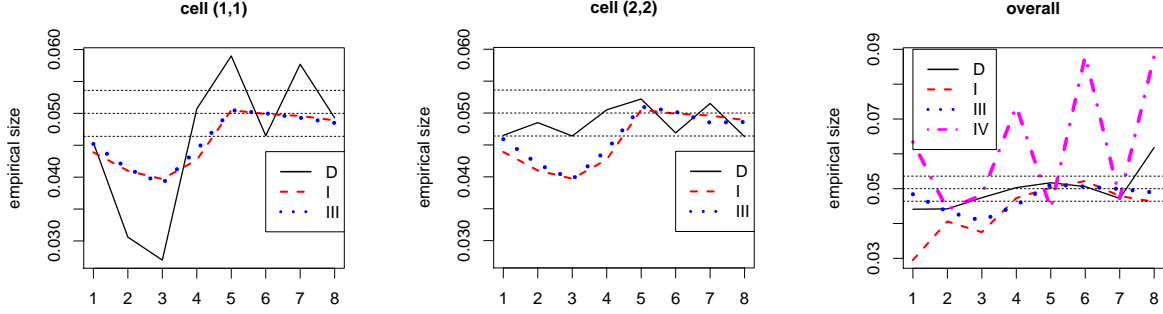


Figure 1: The empirical size estimates of the cell-specific tests for cells (1,1) (left), cell (2,2) (middle), and overall segregation test (right) under the CSR independence pattern in the two-class case. The horizontal lines are located at .0464 (upper threshold for conservativeness), .0500 (nominal level), and .0536 (lower threshold for liberalness). The horizontal axis labels: 1=(10,10), 2=(10,30), 3=(10,50), 4=(30,30), 5=(30,50), 6=(50,50), 7=(50,100), 8=(100,100). The legend labeling: D= Dixon's, I= type I, III= type III, and IV=type IV cell-specific or overall tests.

For the overall tests, Dixon's test and type II test are very similar in size performance (hence only Dixon's test is presented). Type I overall test is conservative for smaller samples, while it has the desired level for larger samples. Dixon's, types I and III are closer to the nominal level, while they are slightly conservative for smaller samples. Type IV overall test has the most unstable behavior, it is extremely liberal for balanced sample sizes, while has the desired level for unbalanced sample sizes. In general Dixon's, type I, or type III overall tests are recommended in the two class case.

## 5.2 Empirical Significance Levels under RL of Two Classes

For the RL pattern we consider three cases, in each of which, we first determine the locations of points and then assign labels to them randomly. See Ceyhan (2010) for more detail. We generate  $n_1$  points iid  $\mathcal{U}(S_1)$  and  $n_2$  points iid  $\mathcal{U}(S_2)$  for the same combinations of  $n_1, n_2$  as in CSR independence case. The locations of these points are taken to be the fixed locations for which we assign the labels randomly. For each sample size combination  $(n_1, n_2)$ , we randomly choose  $n_1$  points (without replacement) and label them as  $X$  points and the remaining  $n_2$  points as  $Y$  points. We repeat the RL procedure  $N_{mc} = 10000$  times for each sample size combination. Empirical sizes are estimated as in the CSR independence case.

In RL case (1), we have  $S_1 = S_2 = (0, 1) \times (0, 1)$  (i.e., the unit square), in RL case (2),  $S_1 = (0, 2/3) \times (0, 2/3)$  and  $S_2 = (1/3, 1) \times (1/3, 1)$ , and in RL case (3),  $S_1 = (0, 1) \times (0, 1)$  and  $S_2 = (2, 3) \times (0, 1)$ .

The locations for which the RL procedure is applied in RL cases (1)-(3) are plotted in Figure 2 for  $n_1 = n_2 = 100$ . Observe that in RL case (1), the set of points are iid  $\mathcal{U}((0, 1) \times (0, 1))$ , i.e., it can be assumed to be from a Poisson process in the unit square. The set of locations are from two overlapping clusters in RL case (2), and from two disjoint clusters in RL case (3).

We present the empirical significance levels for the NNCT-tests under the RL cases (1)-(3) in Figure 3. Under RL cases (1)-(3), for cell (1, 1), type I and III cell-specific tests are closer to the desired size compared to Dixon's cell-specific tests, which is severely conservative when the cell size is small. For cell (2, 2), type I and III have similar performance as in cell (1, 1), while due to the increase in expected cell counts, Dixon's test is closer to desired size. In both cells, the tests are about the desired level for larger sample sizes. For the overall test, Dixon's test and type II tests have very similar size estimates (hence only Dixon's test is presented). Type IV overall test is severely liberal for balanced sample sizes, while the other tests seem to be closer to the desired level, with type III overall test having the best performance.

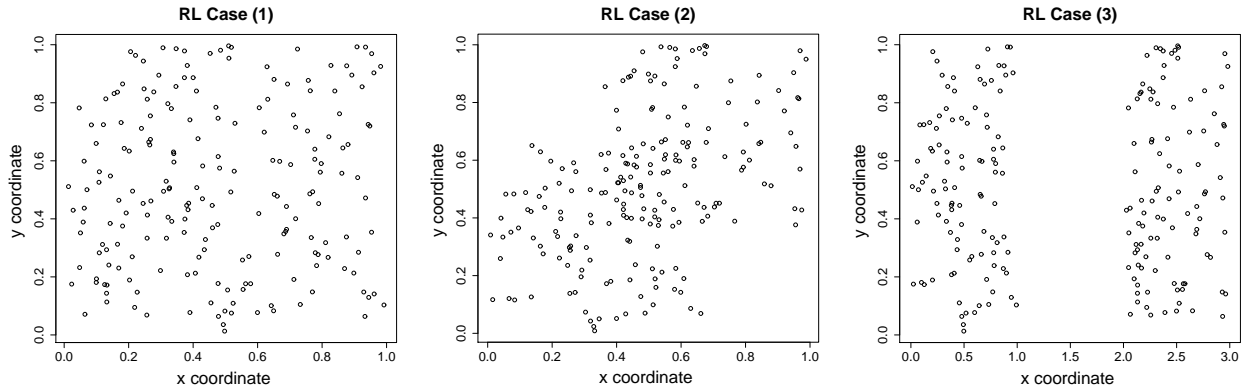


Figure 2: The fixed locations for which RL procedure is applied for RL cases (1)-(3) with  $n_1 = n_2 = 100$  in the two-class case. Notice that  $x$ -axis for RL case (3) is differently scaled.

## 6 Empirical Significance Levels in the Three-Class Case

In this section, we provide the empirical significance levels for Dixon's and the new overall and cell-specific segregation tests in the three-class case under RL and CSR independence patterns.

### 6.1 Empirical Significance Levels under CSR Independence of Three Classes

The symmetry in cell counts for rows in Dixon's cell-specific tests and columns in the new cell-specific tests occur only in the two-class case. To better evaluate the performance of the cell-specific and overall tests, we also consider the three-class case. In the three-class case, we label the classes as  $X$ ,  $Y$ , and  $Z$  or class 1, class 2, and class 3 interchangeably. We generate  $n_1$ ,  $n_2$ ,  $n_3$  points distributed independently uniformly on the unit square  $(0, 1) \times (0, 1)$  from these classes. We use

$$(n_1, n_2, n_3) \in \{(10, 10, 10), (10, 10, 30), (10, 10, 50), (10, 30, 30), (10, 30, 50), (30, 30, 30), (10, 50, 50), (30, 30, 50), (30, 50, 50), (50, 50, 50), (50, 50, 100), (50, 100, 100), (100, 100, 100)\};$$

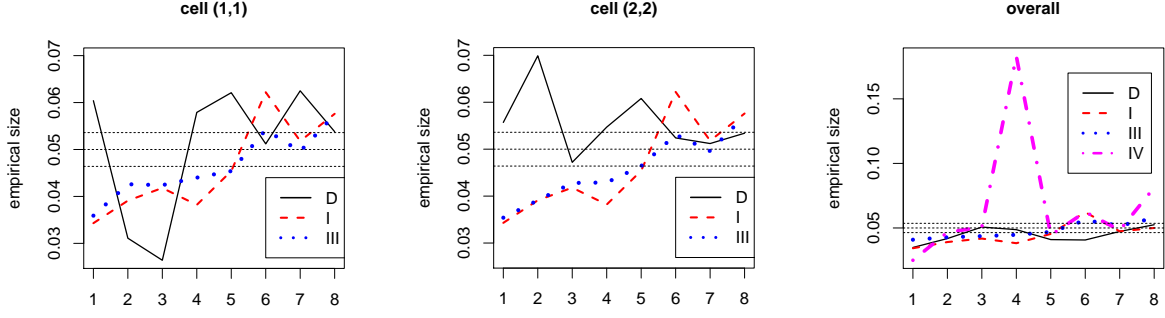
and  $N_{mc} = 10000$ . The empirical sizes and the significance of their deviation from .05 are calculated as in Section 5.1.

We present the empirical significance levels for the cell-specific tests in Figure 4 and for the overall tests in Figure 5. For the cell-specific tests, clearly, type I and III tests are closer to the desired level, and are less affected by the differences in sample sizes. On the other hand, Dixon's test is extremely liberal or conservative, when sample sizes are very different (which may result in smaller expected cell counts). For the overall tests, Dixon's, type II and III are closer to the nominal level, with type III being the closest. On the other hand, type I and IV have opposite performances, in the sense that when one is liberal the other is conservative and vice versa. In particular, type IV (type I) is liberal (conservative) when sample sizes are very different and conservative (liberal) for similar sample sizes.

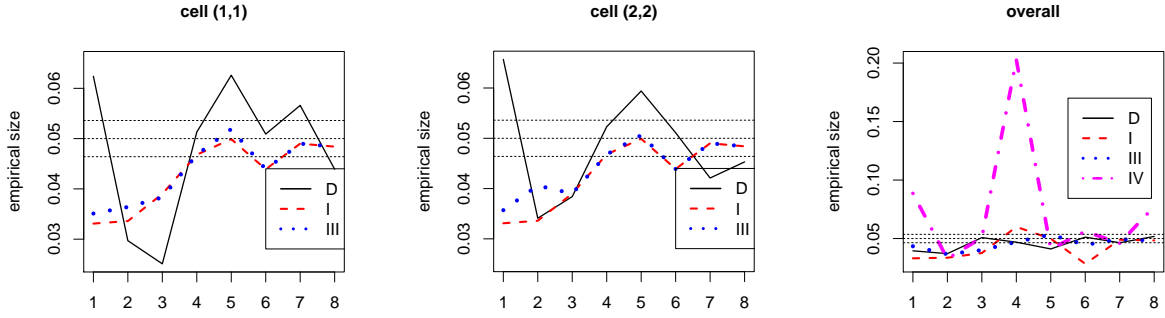
### 6.2 Empirical Significance Levels under RL of Three Classes

We also perform Monte Carlo simulations under RL for the three class case to compare the tests without conditioning on  $Q$  and  $R$ . Under RL, we consider two cases, in each of which we first determine the locations of the points, and then assign the labels randomly. We generate  $n_1$  points iid  $\mathcal{U}(S_1)$ ,  $n_2$  points iid  $\mathcal{U}(S_2)$ , and  $n_3$  points iid  $\mathcal{U}(S_3)$  for each combination of  $n_1, n_2, n_3$  as in CSR independence. The locations of these points are taken to be the fixed and we assign the labels randomly. For each sample size combination  $(n_1, n_2, n_3)$  we pick  $n_1$  points (without replacement) and label them as  $X$ , pick  $n_2$  points from the remaining points (without replacement) and label them as  $Y$  points, and label the remaining  $n_3$  points as  $Z$  points. We estimate the

Empirical Size Plots for the NNCT-Tests for Two Classes under RL Case (1)



RL Case (2)



RL Case (3)

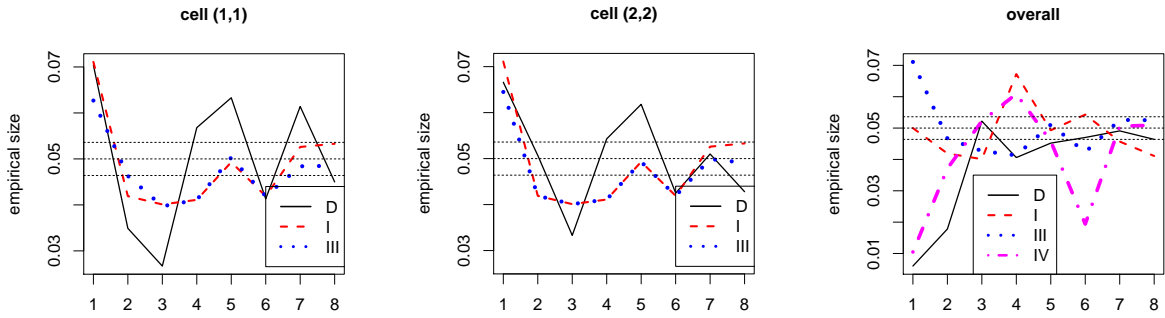


Figure 3: The empirical size estimates of the cell-specific tests for cells (1,1) (left) and (2,2) (middle) and overall segregation test (right) under the RL cases (1)-(3) in the two-class case. The horizontal lines, axis labels, and legend labeling are as in Figure 1.

# Empirical Size Plots for the Cell-Specific Tests under CSR Independence

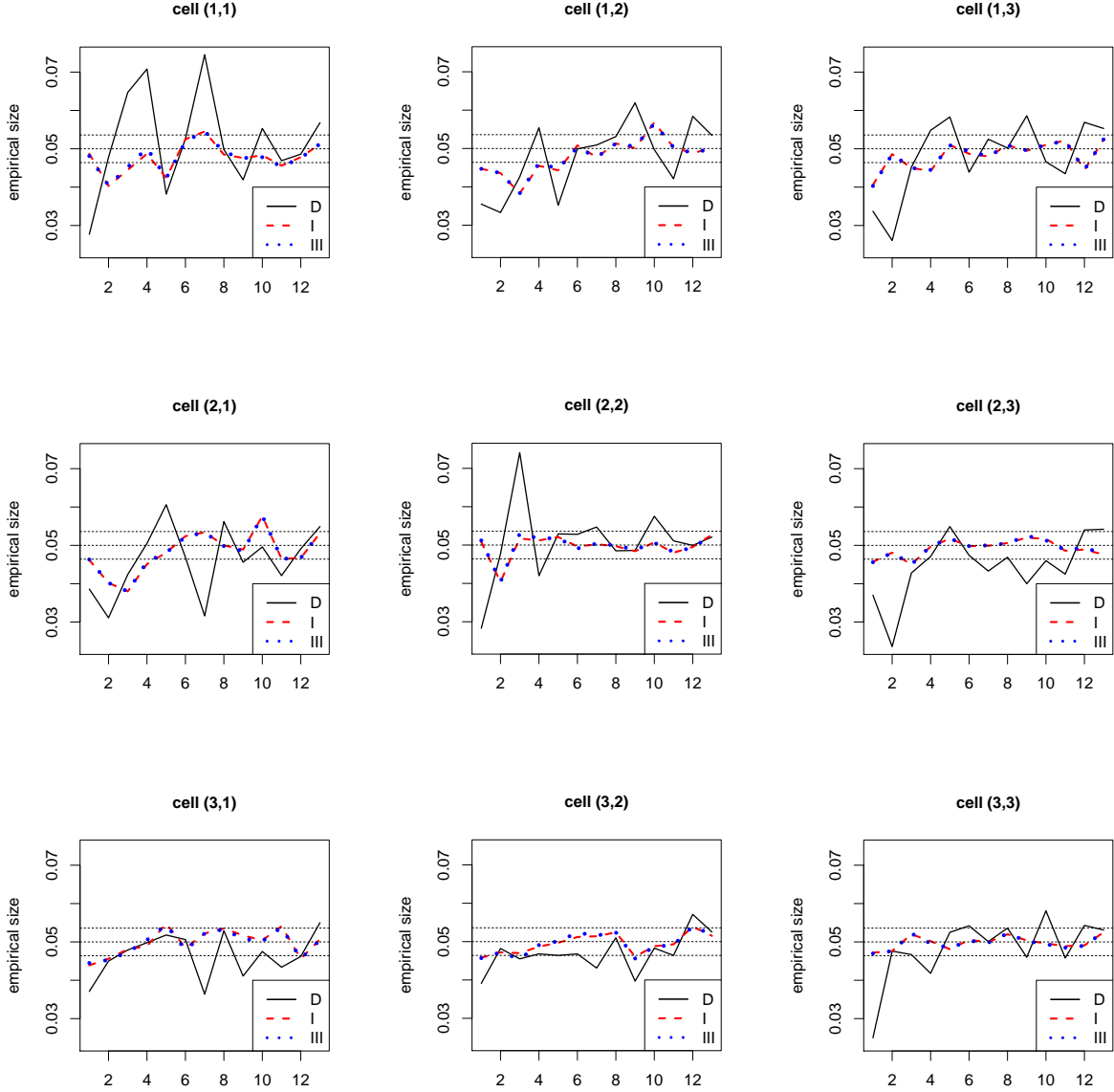


Figure 4: The empirical size estimates of the cell-specific tests for cells (1,1) – (3,3) under the CSR independence pattern in the three-class case. The horizontal lines and legend labeling are as in Figure 1. The horizontal axis labels are: 1=(10,10,10), 2=(10,10,30), 3=(10,10,50), 4=(10,30,30), 5=(10,30,50), 6=(30,30,30), 7=(10,50,50), 8=(30,30,50), 9=(30,50,50), 10=(50,50,50), 11=(50,50,100), 12=(50,100,100), 13=(100,100,100).



## Empirical Size Plots for the Overall Tests under CSR Independence

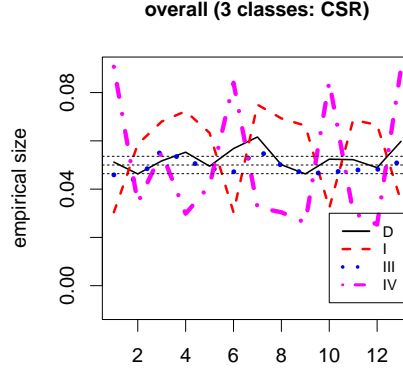


Figure 5: The empirical size estimates of the overall tests under the CSR independence pattern in the three-class case. The horizontal lines, and legend labeling are as in Figure 1 and axis labels are as in Figure 4.

empirical size estimates based on  $N_{mc} = 10000$  replications for each sample size combination as in the CSR independence case.

In RL case (1), we take  $S_1 = S_2 = S_3 = (0, 1) \times (0, 1)$ , and in RL case (2),  $S_1 = (0, 1) \times (0, 1)$ ,  $S_2 = (2, 3) \times (0, 1)$ , and  $S_3 = (1, 2) \times (2, 3)$ . The locations for which the RL procedure is applied in RL cases (1) and (2) are plotted in Figure 6 for  $n_1 = n_2 = n_3 = 100$ . In RL case (1), the locations of the points can be assumed to be from a Poisson process in the unit square. In RL case (2), the locations of the points are from three disjoint clusters.

We present the empirical significance levels under RL case 1 in Figure 7 and under RL case 2 in Figure 8. Under both RL cases, type I and III cell-specific tests perform better in terms of empirical size (i.e., their empirical sizes are closer to the desired level) and less severely affected by smaller cell counts and unbalanced sample sizes, compared to Dixon's cell-specific test. Empirical sizes for the overall tests under RL cases 1 and 2 are presented in Figure 9. Dixon's, type I and III cell-specific tests are closer to the nominal level with type III being the closest. Furthermore, type I and IV exhibit the performance opposite to one another as in the CSR independence case.

## 7 Empirical Power Analysis in the Two-Class Case

We consider three cases for each of segregation and association alternatives in the two-class case.

### 7.1 Empirical Power Analysis under Segregation of Two Classes

Under the segregation alternatives, we generate  $X_i \stackrel{iid}{\sim} \mathcal{U}(S_1)$  and  $Y_j \stackrel{iid}{\sim} \mathcal{U}(S_2)$  where  $S_1 = (0, 1 - s) \times (0, 1 - s)$  and  $S_2 = (s, 1) \times (0, 1)$  for  $i = 1, \dots, n_1$  and  $j = 1, \dots, n_2$  and  $s \in (0, 1)$ . We consider the following three segregation alternatives:

$$H_S^I : s = 1/6, \quad H_S^{II} : s = 1/4, \quad \text{and} \quad H_S^{III} : s = 1/3. \quad (30)$$

Notice that, the level of segregation increases as  $s$  increase; that is, segregation gets stronger from  $H_S^I$  to  $H_S^{III}$ . We calculate the power estimates using the asymptotic critical values based on the standard normal distribution for the cell-specific tests and the corresponding  $\chi^2$ -distributions for the overall tests.

The power estimates based on the asymptotic critical values are presented in Figure 10. We omit the



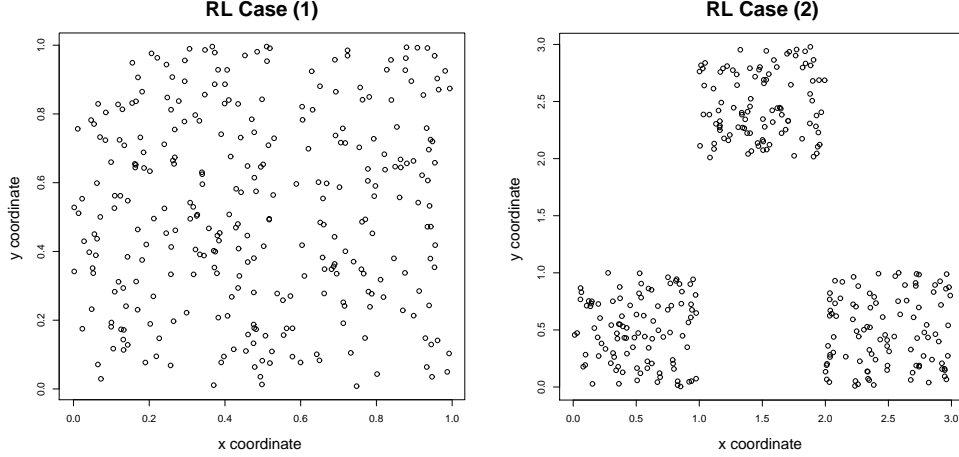


Figure 6: The fixed locations for which RL procedure is applied for RL cases (1) and (2) with  $n_1 = n_2 = n_3 = 100$  in the two-class case. Notice that  $x$ -axis for RL case (2) is differently scaled.

power estimates of the cell-specific tests for cells (1,2) and (2,1), since they would be same as cells (1,1) and (2,2) (but in the reverse direction). As expected, the power estimates increase as segregation gets stronger and also as sample size increases. For the cell-specific and overall tests, type I and III tests have the highest power estimates. Dixon's and type II have very similar but lower power estimates, and the lowest power estimates are with type IV overall test.

## 7.2 Empirical Power Analysis under Association of Two Classes

Under the association alternatives, we consider three cases also. In each case, we generate  $X_i \stackrel{iid}{\sim} \mathcal{U}((0,1) \times (0,1))$  for  $i = 1, 2, \dots, n_1$ . Then we generate  $Y_j$  associated with  $X$ 's for  $j = 1, 2, \dots, n_2$  as follows. For each  $j$ , select an  $i$  randomly, and set  $Y_j = X_i + R_j (\cos T_j, \sin T_j)'$  where  $R_j \stackrel{iid}{\sim} \mathcal{U}(0, r)$  with  $r \in (0, 1)$  and  $T_j \stackrel{iid}{\sim} \mathcal{U}(0, 2\pi)$ . We consider the following association alternatives:

$$H_A^I : r = 1/4, \quad H_A^{II} : r = 1/7, \quad \text{and} \quad H_A^{III} : r = 1/10. \quad (31)$$

Notice that association gets stronger as  $r$  decreases; that is, association gets stronger from  $H_A^I$  to  $H_A^{III}$ . Furthermore, by construction, the association of  $Y$  points with  $X$  points is stronger, compared to the association of  $X$  points with  $Y$  points.

The empirical power estimates under association are presented in Figure 11. As expected as association gets stronger, the power estimates increase. However, there is no clear trend as total sample size  $n$  increases, since, by construction, association alternative depends on the sample size differences. For cell (1,1), type I and III cell-specific tests have higher power estimates, while for cell (2,2) Dixon's test has higher power estimates for weak association and smaller sample sizes.

## 8 Empirical Power Analysis in the Three-Class Case

We also consider three cases for each of segregation and association alternatives in the three-class case.

### 8.1 Empirical Power Analysis under Segregation of Three Classes

Under the segregation alternatives, we generate  $X_i \stackrel{iid}{\sim} \mathcal{U}(S_1)$ ,  $Y_j \stackrel{iid}{\sim} \mathcal{U}(S_2)$ , and  $Z_k \stackrel{iid}{\sim} \mathcal{U}(S_3)$  for  $i = 1, \dots, n_1$ ,  $j = 1, \dots, n_2$ , and  $k = 1, \dots, n_3$  where  $S_1 = (0, 1 - 2s) \times (0, 1 - 2s)$ ,  $S_2 = (2s, 1) \times (2s, 1)$ , and  $S_3 =$

Empirical Size Plots for the Cell-Specific Tests under RL case (1)

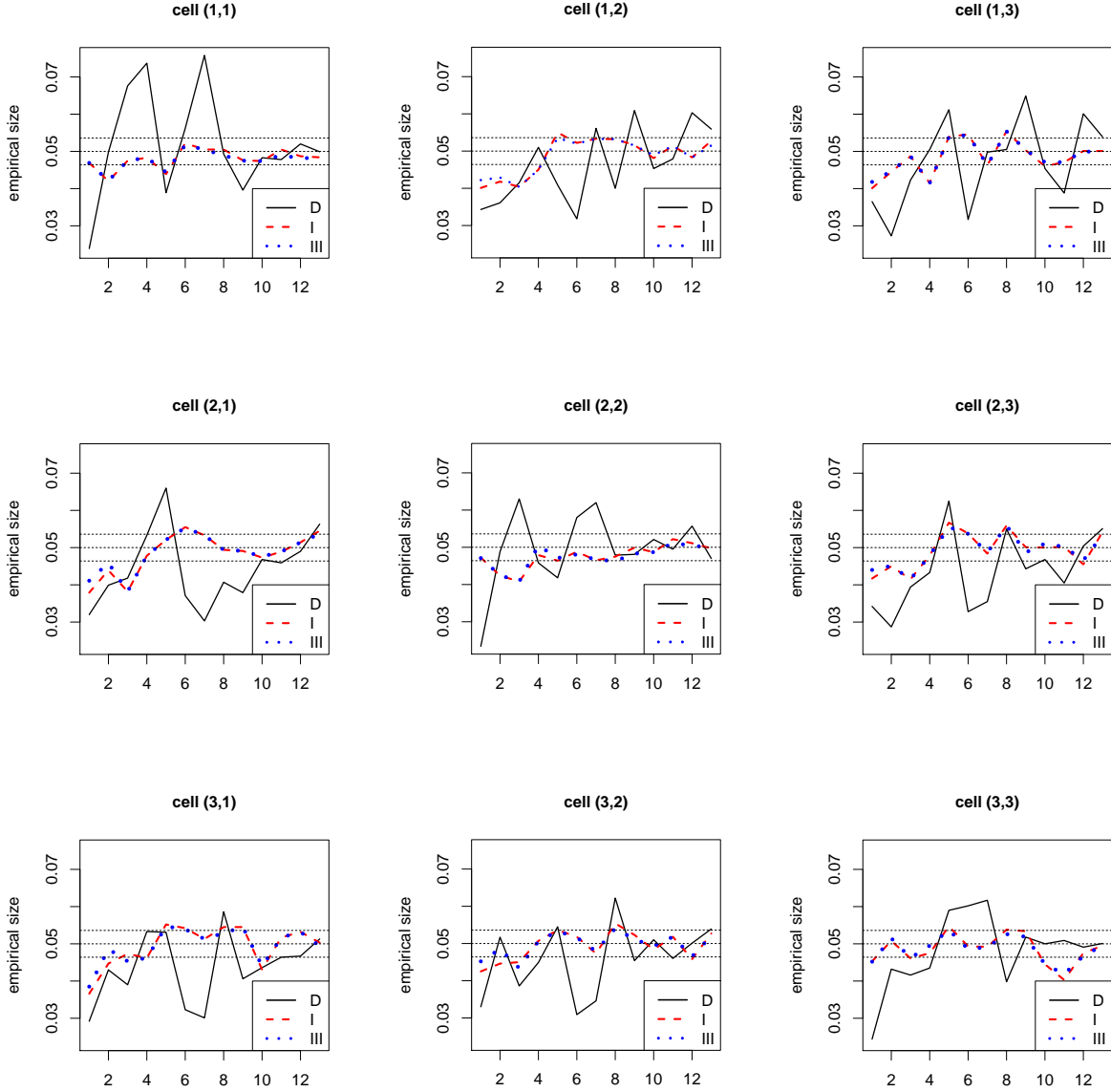


Figure 7: The empirical size estimates of the cell-specific tests for cells (1,1) – (3,3) under the RL case 1 in the three-class case. The horizontal lines and legend labeling are as in Figure 1 and axis labeling are as in Figure 4.

Empirical Size Plots for the Cell-Specific Tests under RL case (2)

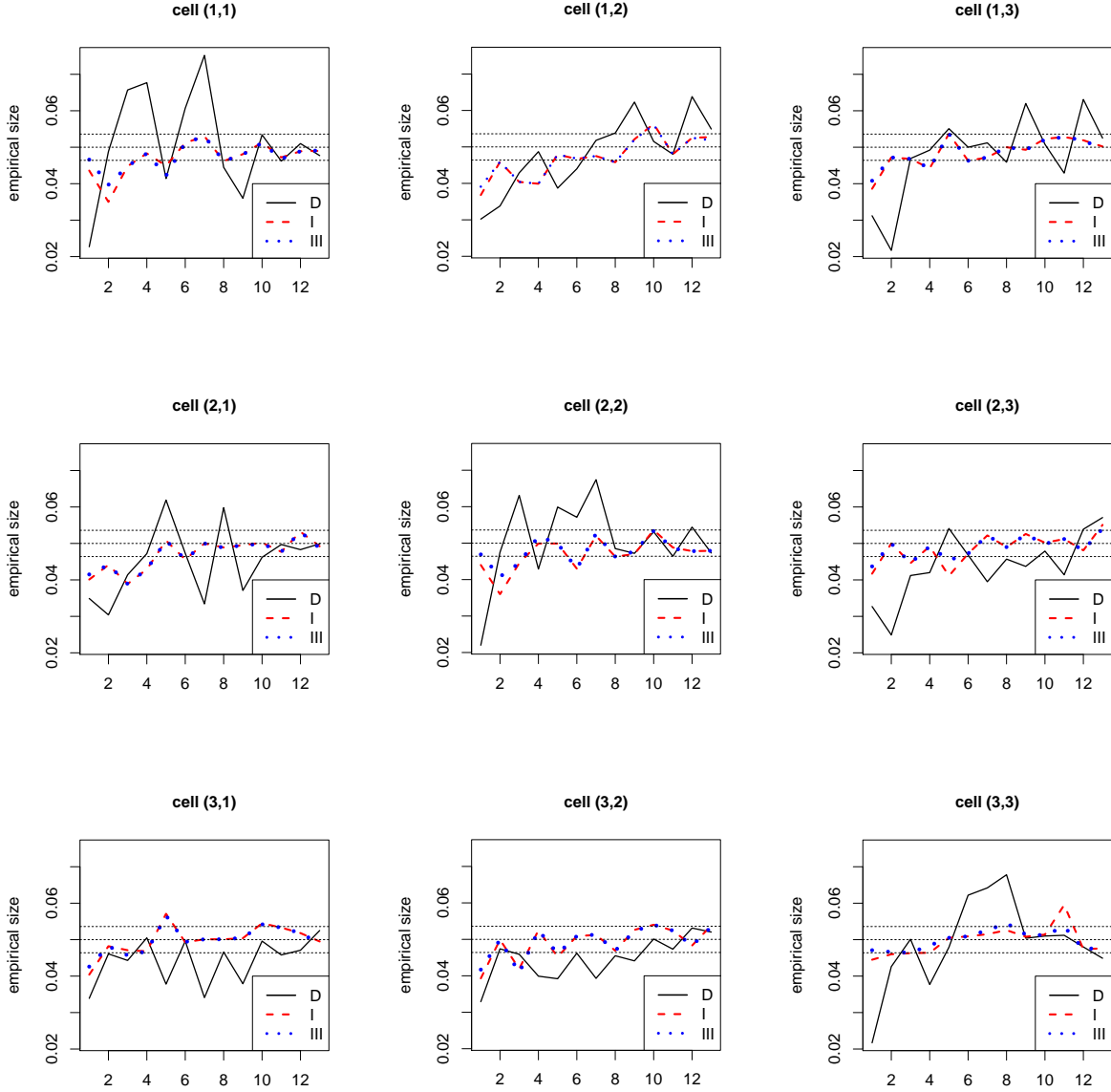


Figure 8: The empirical size estimates of the cell-specific tests for cells (1,1) – (3,3) under the RL case 2 in the three-class case. The horizontal lines and legend labeling are as in Figure 1 and axis labeling are as in Figure 4.

## Empirical Size Plots for the Overall Tests under RL cases 1 and 2

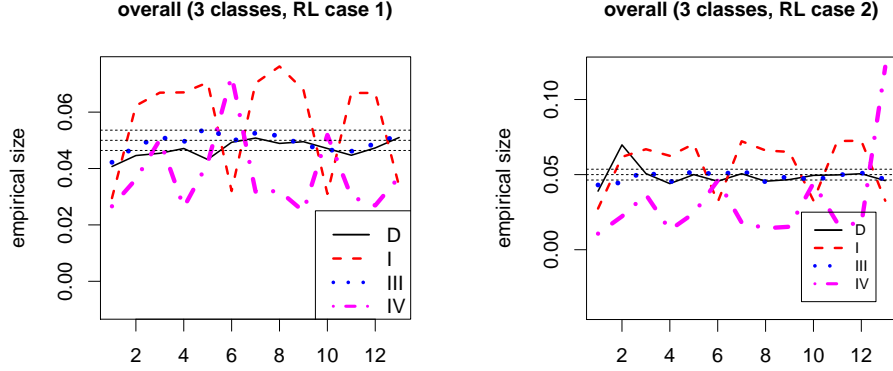


Figure 9: The empirical size estimates of the overall tests under the RL cases 1 and 2 in the three-class case. The horizontal lines and legend labeling are as in Figure 1 and axis labeling are as in Figure 4.

$(s, 1 - s) \times (s, 1 - s)$  with  $s \in (0, 1/2)$ . We consider the following segregation alternatives:

$$H_{S_1} : s = 1/12, \quad H_{S_2} : s = 1/8, \quad \text{and} \quad H_{S_3} : s = 1/6. \quad (32)$$

Notice that, as  $s$  increases, segregation between the classes gets stronger; that is, segregation gets stronger from  $H_{S_1}$  to  $H_{S_3}$ . Furthermore, by construction classes  $X$  and  $Y$  are more segregated compared to  $Z$  and  $X$  or  $Z$  and  $Y$ . In fact, the segregation between  $X$  and  $Z$  and segregation between  $Y$  and  $Z$  are identical (as a stochastic process).

Empirical power estimates for the diagonal cells  $(1, 1)$ ,  $(2, 2)$ , and  $(3, 3)$  under segregation alternatives are plotted in Figure 12 and for the off-diagonal cells  $(1, 2)$ ,  $(1, 3)$ , and  $(2, 3)$  are plotted in Figure 13. For diagonal cells  $(1, 1)$  and  $(2, 2)$  type I and III tests have higher power, while for diagonal cell  $(3, 3)$ , all tests have similar power estimates. For the off-diagonal cells  $(1, 2)$  and  $(1, 3)$  all tests have similar power estimates, while for cell  $(2, 3)$  type I and III tests have higher power. In line with our simulation setup, power estimates for cells  $(1, 1)$  and  $(2, 2)$  are higher compared to cell  $(3, 3)$ , as classes  $X$  and  $Y$  are more segregated compared to class  $Z$ . For the same reason, power estimates for cell  $(1, 2)$  is higher compared to cells  $(1, 3)$  and  $(2, 3)$ .

Empirical power estimates for the overall tests are presented in Figure 14. Dixon's and type II tests have very similar power estimates, while type III test has higher power than these tests. However, type I test is highly dependent on differences in relative abundances of the classes. In particular, for balanced samples, type I test has the lowest power estimates, while for unbalanced samples, type I test has the highest power estimates.

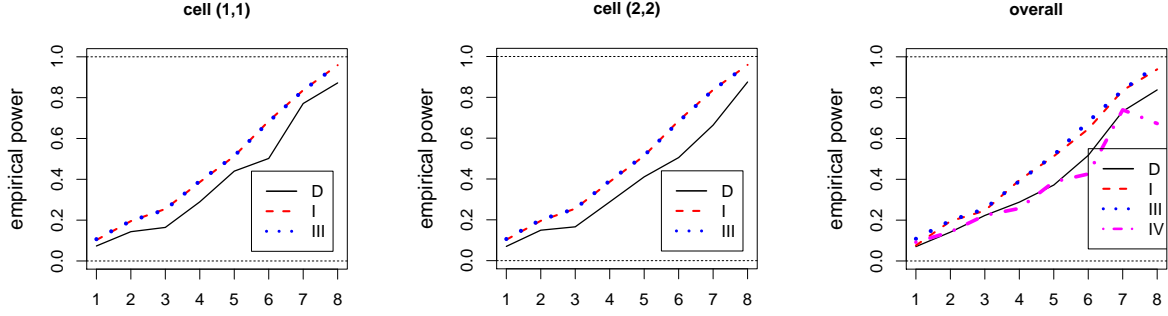
## 8.2 Empirical Power Analysis under Association of Three Classes

Under the association alternatives, we also consider three cases. We generate  $X_i \stackrel{iid}{\sim} \mathcal{U}((0, 1) \times (0, 1))$  for  $i = 1, 2, \dots, n_1$ . Then we generate  $Y_j$  and  $Z_k$  for  $j = 1, 2, \dots, n_2$  and  $k = 1, 2, \dots, n_3$  as follows. For each  $j$ , select an  $i$  randomly, and set  $Y_j := X_i + R_j^Y (\cos T_j, \sin T_j)'$  where  $R_j^Y \stackrel{iid}{\sim} \mathcal{U}(0, r_y)$  with  $r_y \in (0, 1)$  and  $T_j \stackrel{iid}{\sim} \mathcal{U}(0, 2\pi)$ . Similarly, for each  $k$ , select an  $i'$  randomly, and set  $Z_k := X_{i'} + R_k^Z (\cos U_k, \sin U_k)'$  where  $R_k^Z \stackrel{iid}{\sim} \mathcal{U}(0, r_z)$  with  $r_z \in (0, 1)$  and  $U_k \stackrel{iid}{\sim} \mathcal{U}(0, 2\pi)$ . We consider the following association alternatives:

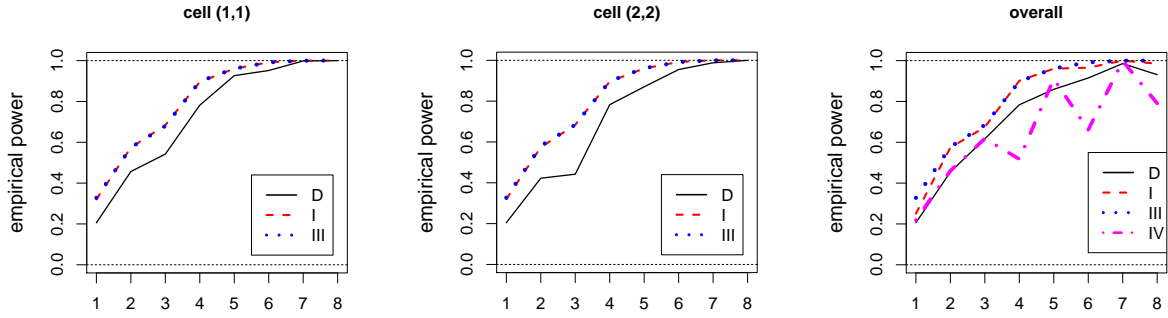
$$H_{A_1} : r_y = 1/7, r_z = 1/10, \quad H_{A_2} : r_y = 1/10, r_z = 1/20, \quad H_{A_3} : r_y = 1/13, r_z = 1/30. \quad (33)$$

As  $r_y$  and  $r_z$  decrease, the level of association increases. That is, the association between  $X$  and  $Y$  and association between  $X$  and  $Z$  get stronger from  $H_{A_1}$  to  $H_{A_3}$ . By construction, classes  $Y$  and  $Z$  are associated

Empirical Power Estimates of the NNCT-Tests under  $H_S^I$



Power Estimates under  $H_S^{II}$



Power Estimates under  $H_S^{III}$

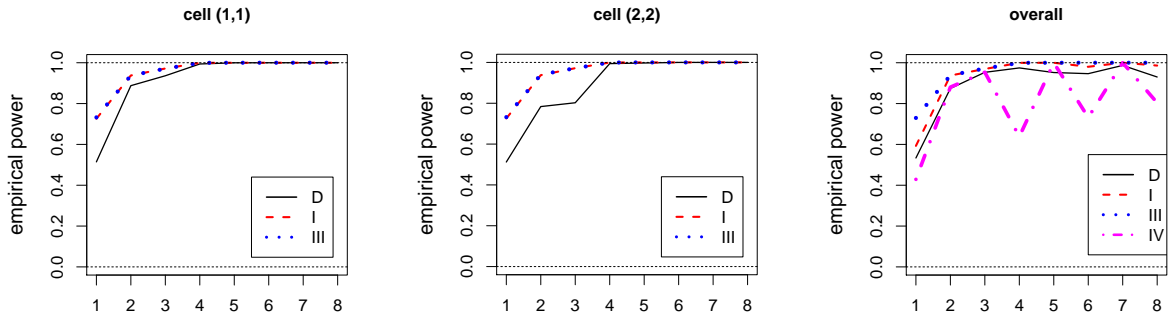
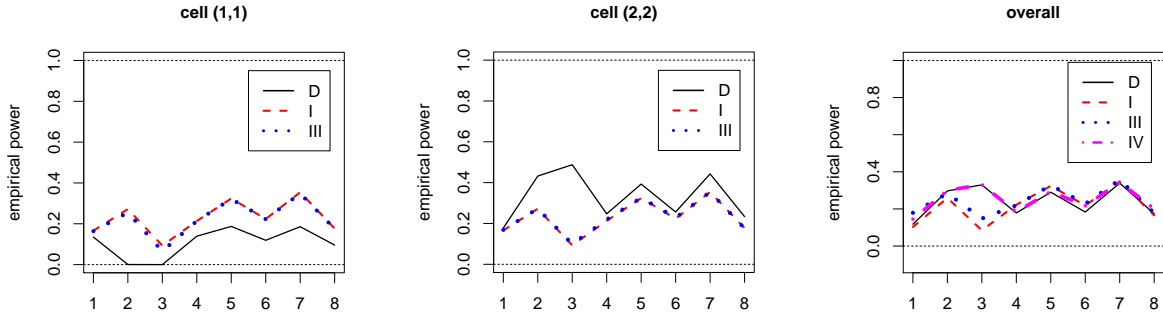
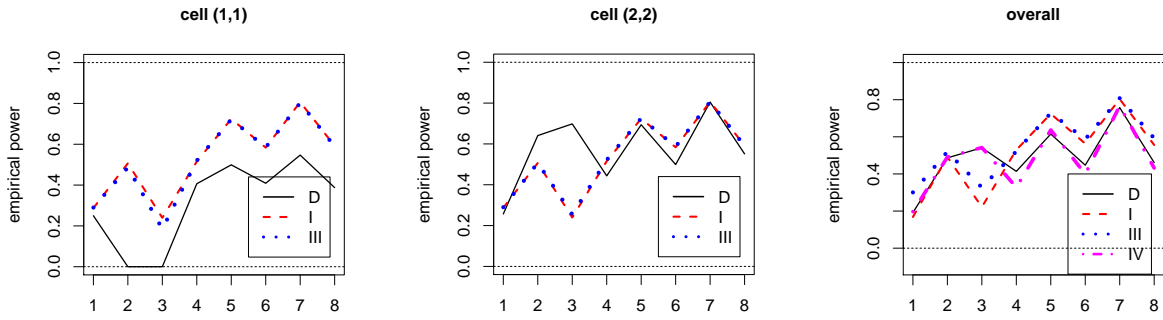


Figure 10: The empirical power estimates for the cell-specific (left and middle columns) and the overall tests (right column) under the segregation alternatives in the two-class case. The horizontal axis labels and legend are as in Figure 1.

### Empirical Power Estimates of the NNCT-Tests under $H_A^I$



### Power Estimates under $H_A^{II}$



### Power Estimates under $H_A^{III}$

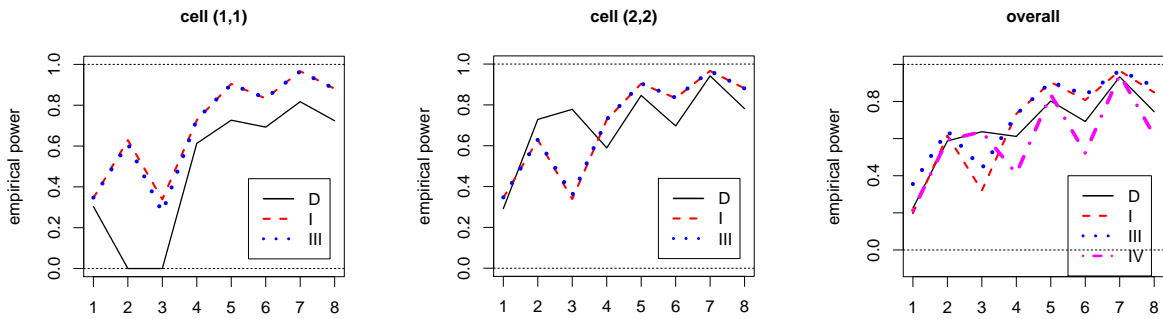
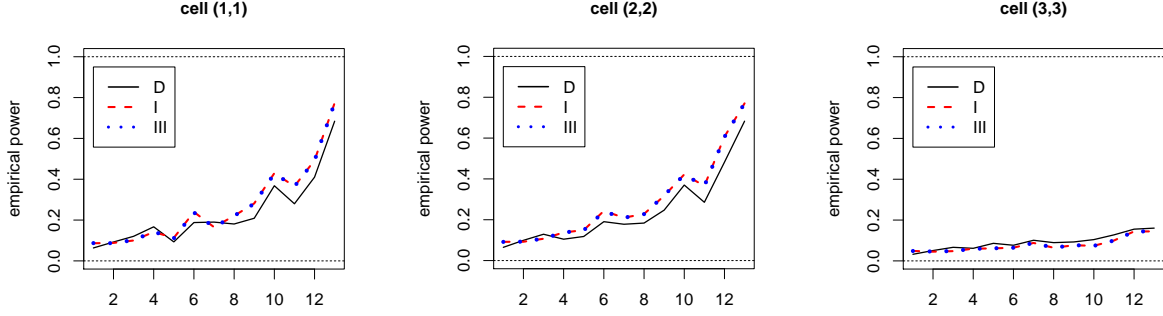
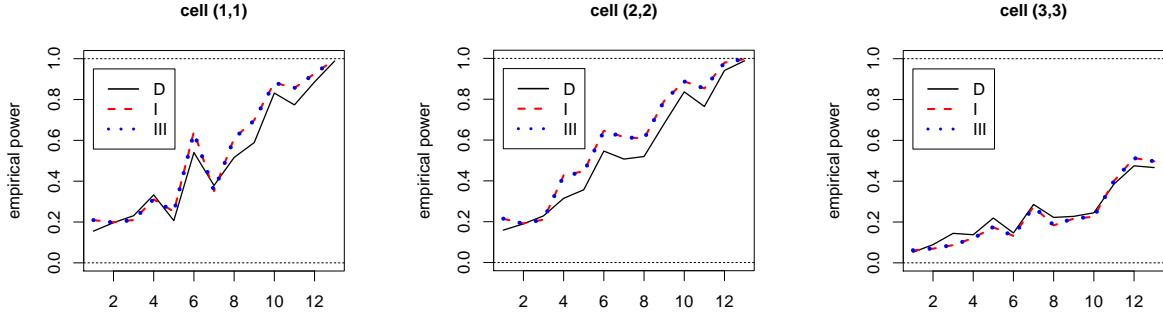


Figure 11: The empirical power estimates for the NNCT-tests under the association alternatives in the two-class case. The horizontal axis labels and legend labeling are as in Figure 1.

### Empirical Power Estimates of Cell-Specific Tests under $H_{S_1}$



### Power Estimates under $H_{S_2}$



### Power Estimates under $H_{S_3}$

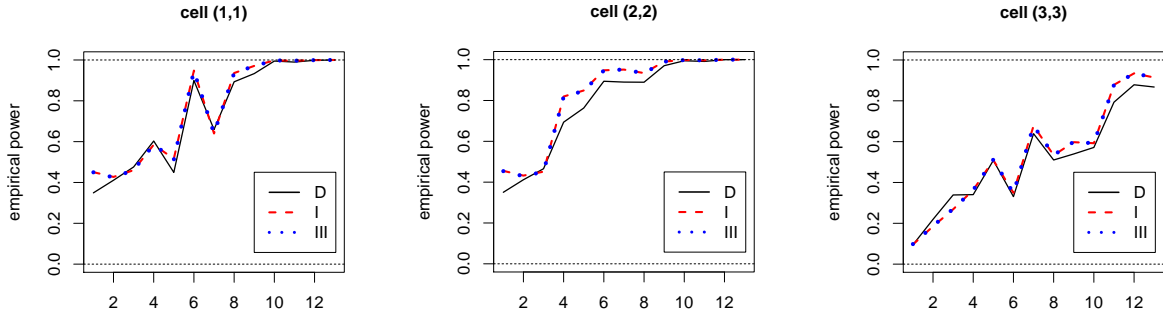
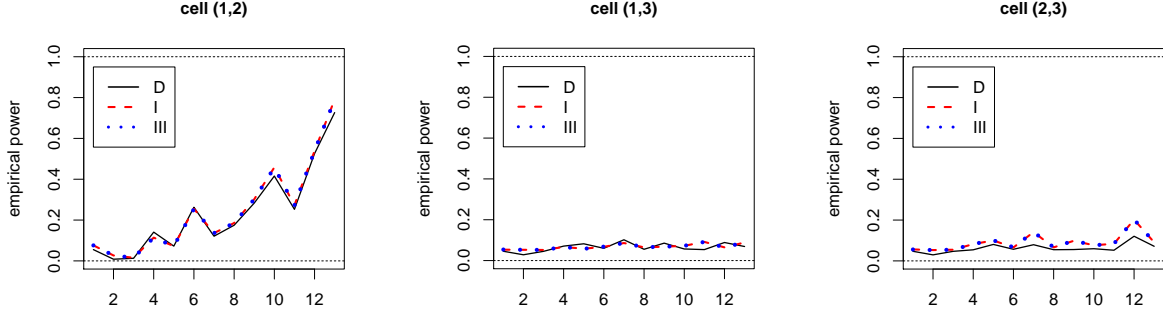
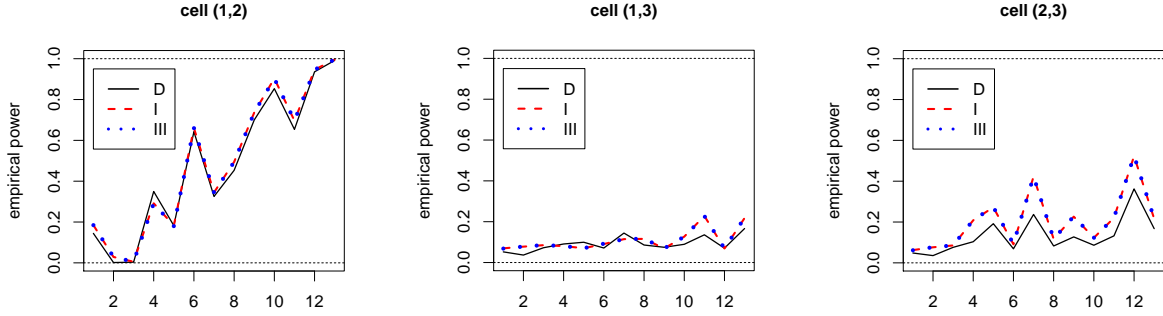


Figure 12: The empirical power estimates of the cell-specific tests for cells (1,1), (2,2), and (3,3) under the segregation alternatives  $H_{S_1}$  (top),  $H_{S_2}$  (middle), and  $H_{S_3}$  (bottom) in the three-class case. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.

### Empirical Power Estimates of Cell-Specific Tests under $H_{S_1}$



### Power Estimates under $H_{S_2}$



### Power Estimates under $H_{S_3}$

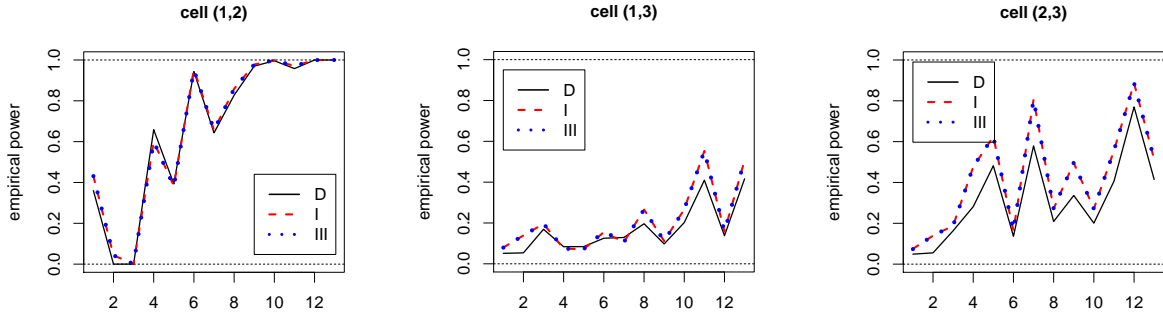


Figure 13: The empirical power estimates of the cell-specific tests for cells (1,2), (1,3), and (2,3) under the segregation alternatives  $H_{S_1}$  (top),  $H_{S_2}$  (middle), and  $H_{S_3}$  (bottom) in the three-class case. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.



## Empirical Power Estimates of Overall Tests under $H_S$

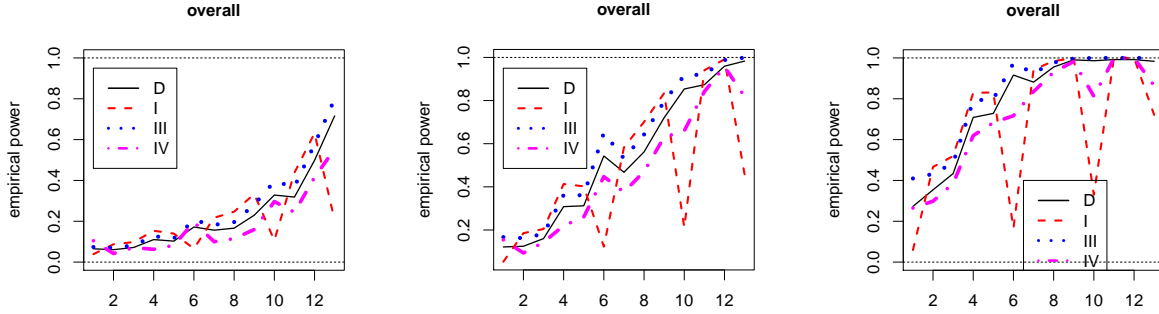


Figure 14: The empirical power estimates of the overall tests under the segregation alternatives  $H_{S_1}$  (left),  $H_{S_2}$  (middle), and  $H_{S_3}$  (right) in the three-class case. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.

with class  $X$ , while classes  $Y$  and  $Z$  are not associated, but perhaps mildly segregated for small  $r_y$  and  $r_z$ . Furthermore, by construction, classes  $X$  and  $Z$  are more associated compared to classes  $X$  and  $Y$ .

The empirical power estimates for cells (1, 2) and (2, 1) are presented in Figure 15, and for cells (1, 3) and (3, 1) are presented in Figure 16. For cells (1, 2) and (1, 3), type I and III cell-specific tests have higher power, while for cells (2, 1) and (3, 1), Dixon's cell-specific test has higher power. The power estimates for the overall tests are presented in Figure 17. For the overall test, there is no clear winner in terms of power. For large samples, Dixon's test, type II and III have similar and larger power, while for smaller samples type IV tends to have higher power estimates.

## 9 Empirical Size and Power Analysis for the One-vs-Rest Type Tests in the Three Class Case

In one-versus-rest type testing, we implement Monte Carlo simulations as in Section 6.1 to assess the empirical size performance of these tests under CSR independence. We present the empirical size estimates for various sample size combinations in Figure 18 where only cell-specific tests for cell (2, 2) and the overall test are presented, since the cell-specific test for cell (1, 1) is the same as in the  $3 \times 3$  NNCT analysis. Among cell-specific tests, types I and III tests perform better compared to Dixon's test, since they are closer to the nominal level for large samples. For the overall tests, except for type IV test, the tests are about the nominal level, but closer to the nominal level at different sample size combinations.

To evaluate the power performance of these tests, we perform simulations under segregation alternatives as in Section 8.1. The empirical power estimates under the three segregation alternatives are presented in Figures 19 and 20. Among the tests, type I and III tests have higher power estimates compared to other types. One class-vs-rest tests for classes 1 and 2 have higher power estimates, compared to that of class 3. This occurs since by construction, classes 1 and 2 are equally segregated from other classes, and these classes are more segregated compared to class 3.

For the association alternatives, we perform the simulations as in Section 8.2. The corresponding power estimates under the three association alternatives are presented in Figures 21 and 22. Under the association alternatives, Dixon's cell-specific test and Dixon's and type IV overall tests have better power performance. Since, by construction, class 1-vs-rest statistics test the association of the other classes with class 1, they have higher power estimates. For classes 1 and 2, Dixon's one class-vs-rest tests have higher power, while for class 3-vs-rest tests have similar power, although type I and III tests have slightly higher power estimates.

# Empirical Power Estimates of Cell-Specific Tests under $H_A$

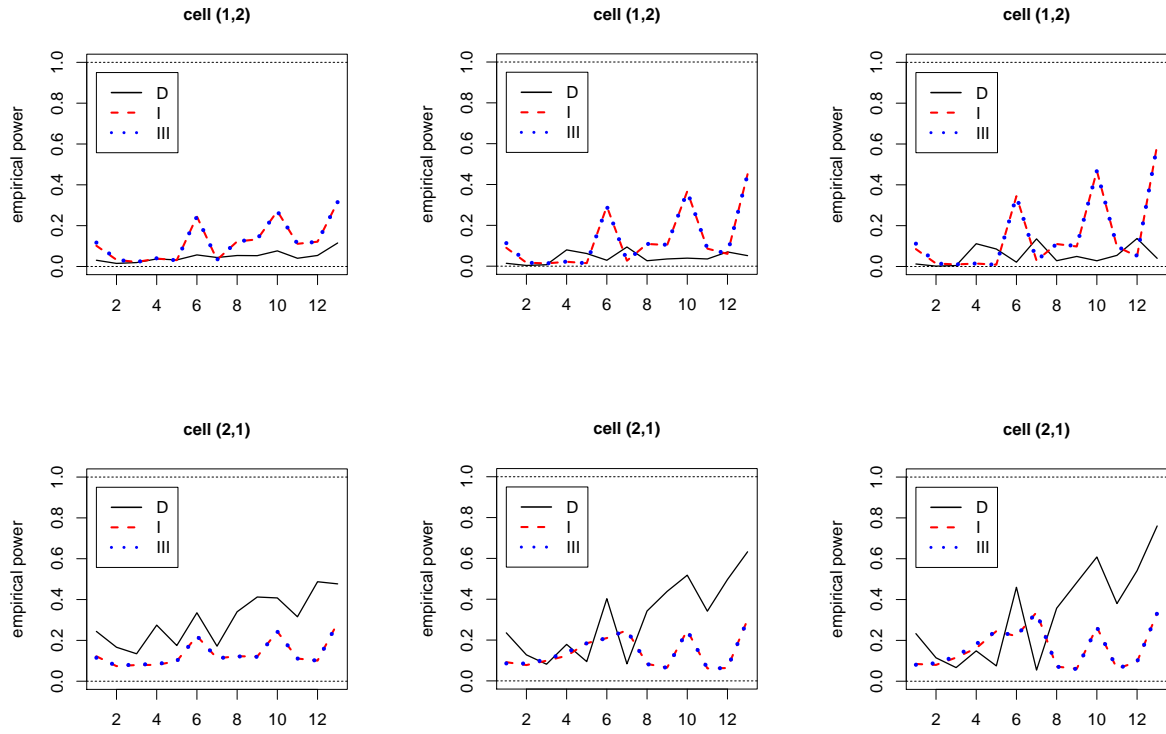


Figure 15: The empirical power estimates of the cell-specific tests for cells (1,2) and (2,1) under the association alternatives  $H_{A_1}$  (left),  $H_{A_2}$  (middle), and  $H_{A_3}$  (right) in the three-class case. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.

### Empirical Power Estimates of Cell-Specific Tests under $H_A$

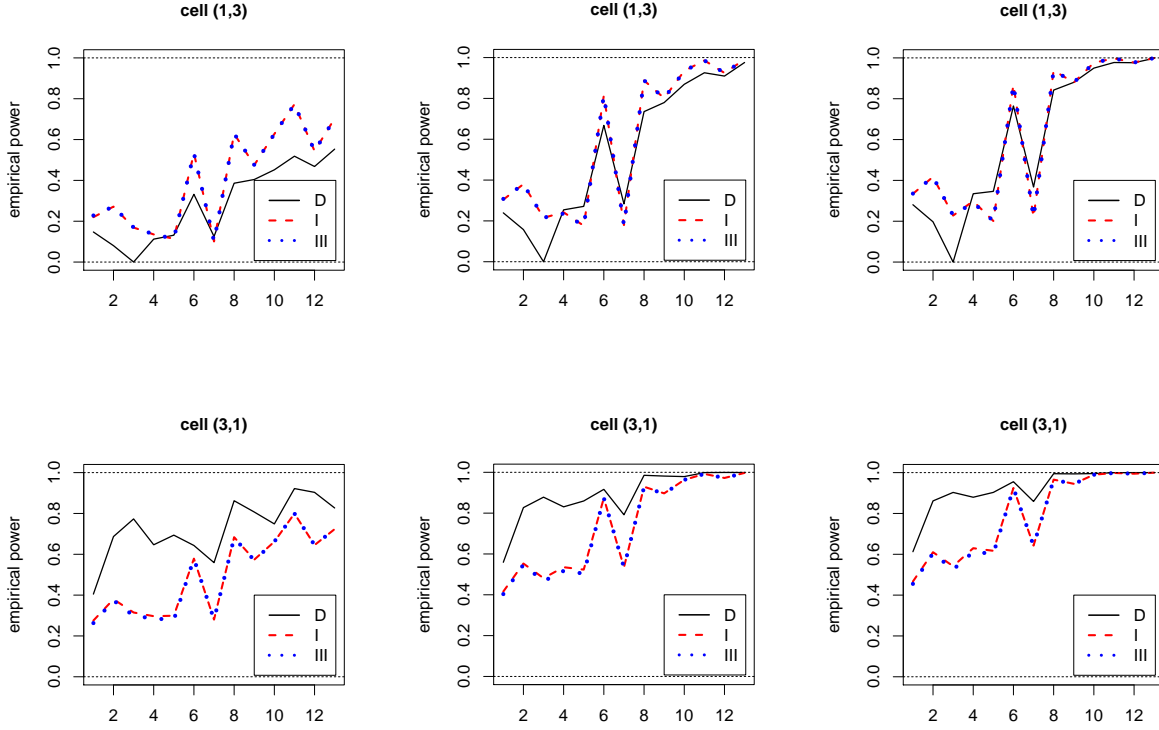


Figure 16: The empirical power estimates of the cell-specific tests for cells (1,3) and (3,1) under the association alternatives  $H_{A_1}$  (left),  $H_{A_2}$  (middle), and  $H_{A_3}$  (right) in the three-class case. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.

### Empirical Power Estimates of Overall Tests under $H_A$

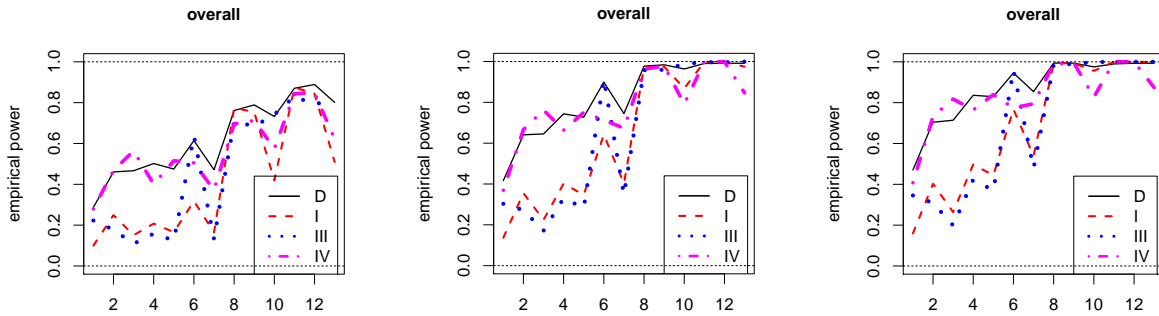
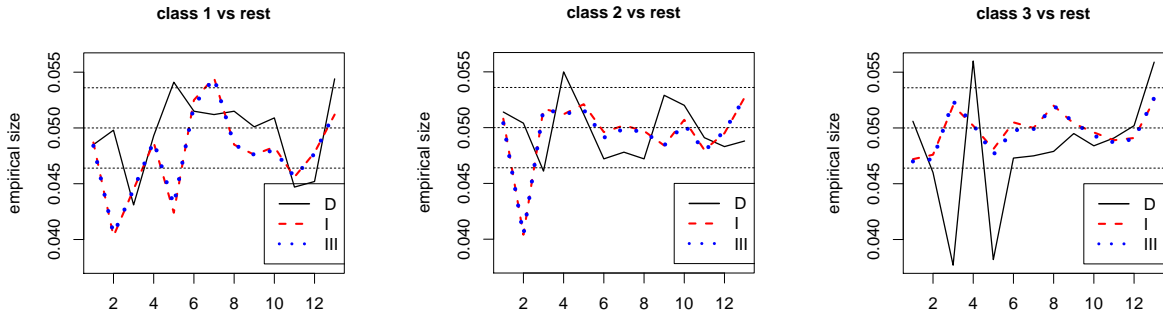


Figure 17: The empirical power estimates of the overall test under the association alternatives  $H_{A_1}$  (left),  $H_{A_2}$  (middle), and  $H_{A_3}$  (right) in the three-class case. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.

### Empirical Size Estimates of Cell-Specific Tests for cell (2, 2) under CSR



### Empirical Size Estimates of Overall Tests under CSR

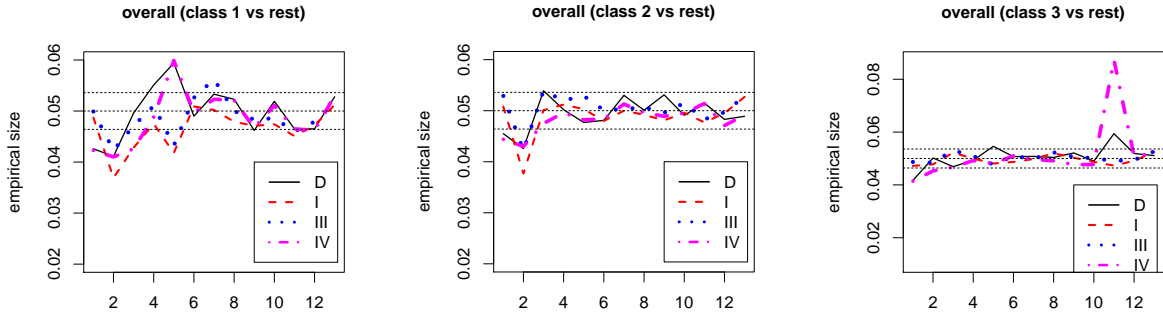
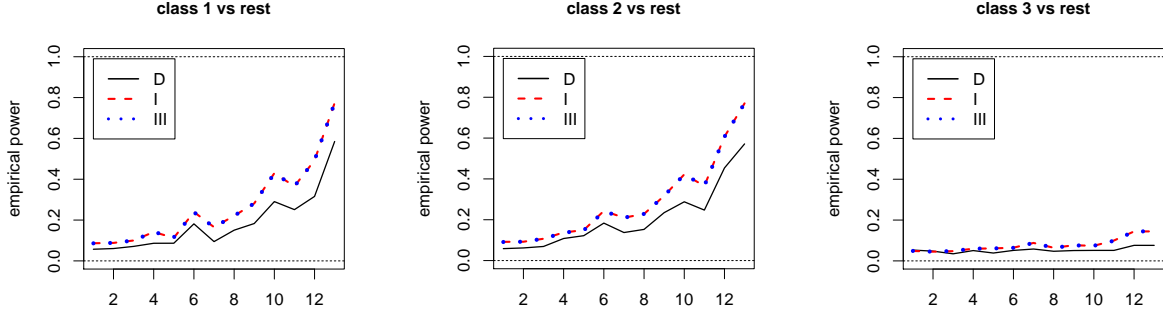
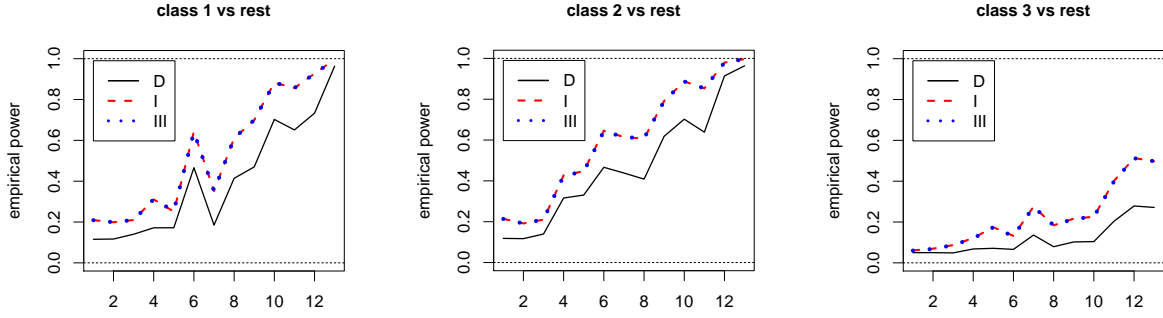


Figure 18: The empirical size estimates of the cell-specific tests for cell (2, 2) and overall tests under CSR independence with one-versus-rest type testing. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.

Empirical Power Estimates of Cell-Specific Tests under  $H_{S_1}$



Power Estimates under  $H_{S_2}$



Power Estimates under  $H_{S_3}$

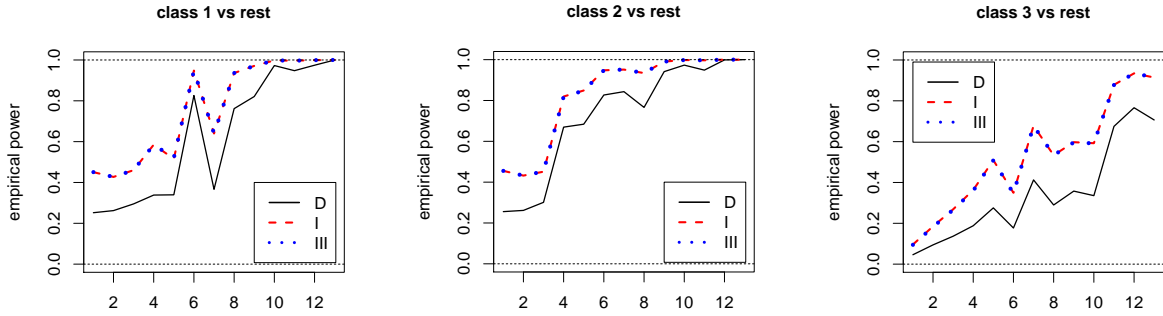
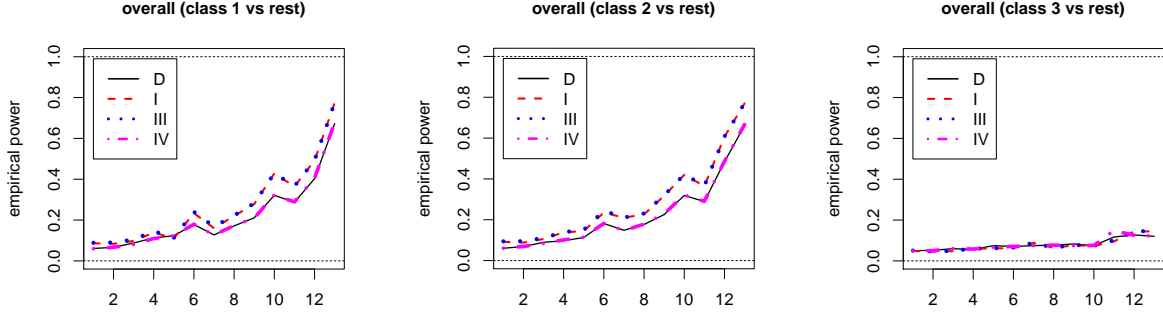
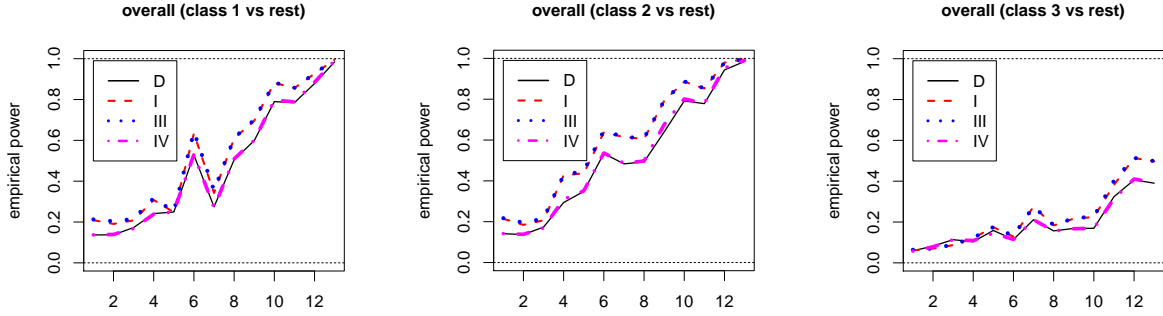


Figure 19: The empirical power estimates of the cell-specific tests for cell (2,2), under the segregation alternatives  $H_{S_1}$  (top),  $H_{S_2}$  (middle), and  $H_{S_3}$  (bottom) in the three-class case with the one-versus-rest type testing. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.

### Empirical Power Estimates of Overall Tests under $H_{S_1}$



### Power Estimates under $H_{S_2}$



### Power Estimates under $H_{S_3}$

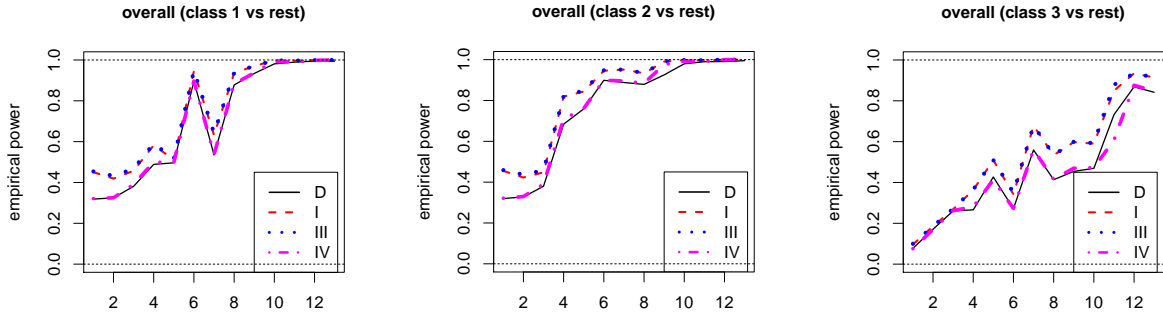
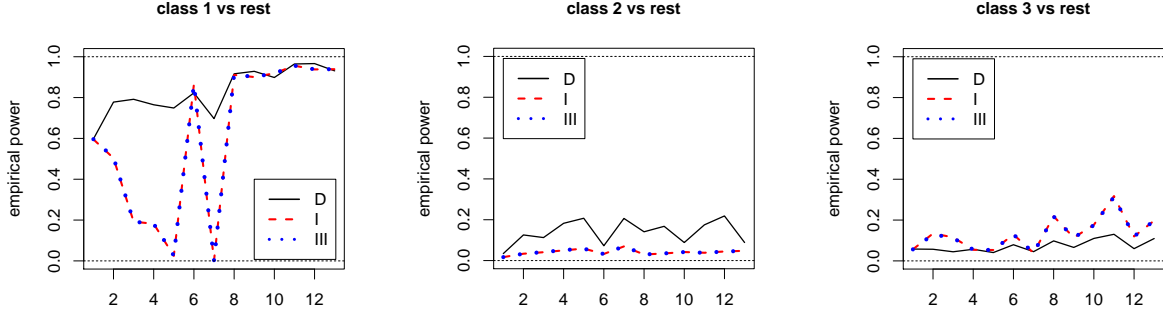
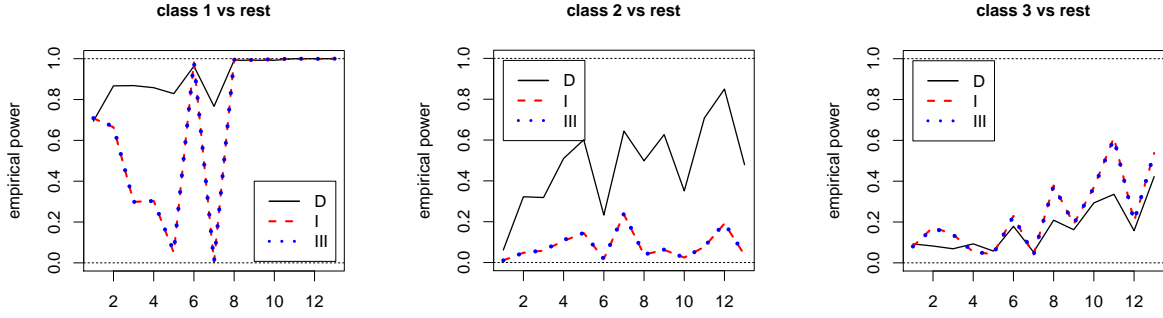


Figure 20: The empirical power estimates of the overall tests under the segregation alternatives  $H_{S_1}$  (top),  $H_{S_2}$  (middle), and  $H_{S_3}$  (bottom) in the three-class case with the one-versus-rest type testing. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.

### Empirical Power Estimates of Cell-Specific Tests under $H_{A_1}$



### Power Estimates under $H_{A_2}$



### Power Estimates under $H_{A_3}$

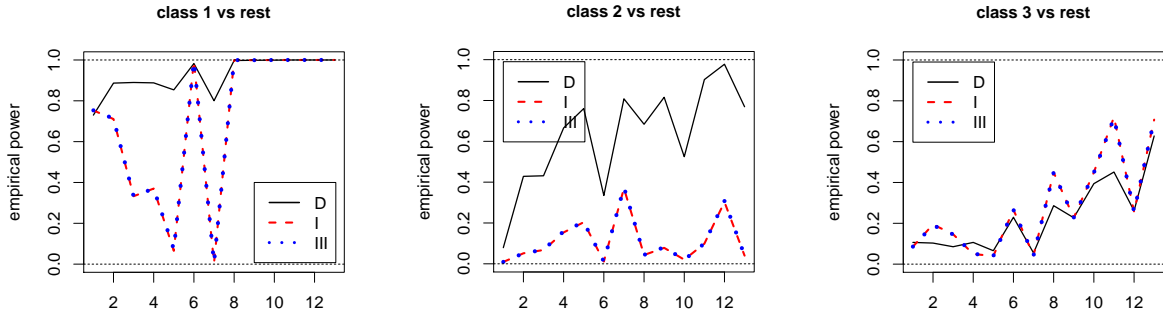
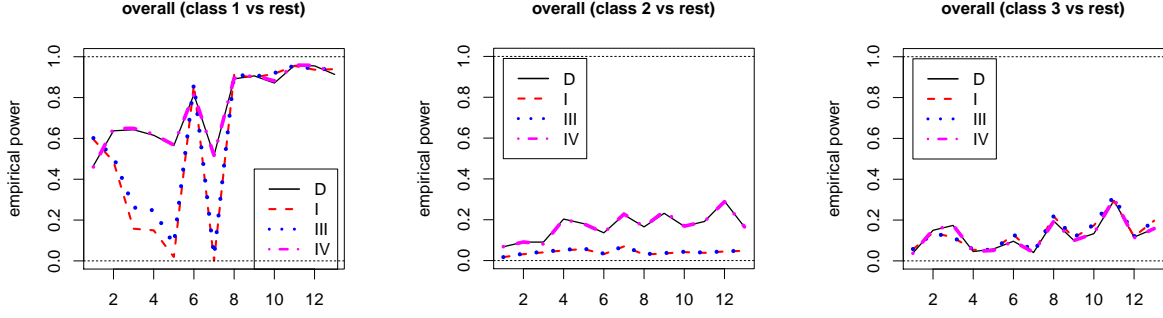


Figure 21: The empirical power estimates of the cell-specific tests for cell (2,2), under the association alternatives  $H_{A_1}$  (top),  $H_{A_2}$  (middle), and  $H_{A_3}$  (bottom) in the three-class case with the one-versus-rest type testing. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.

### Empirical Power Estimates of Overall Tests under $H_{A_1}$



### Power Estimates under $H_{A_2}$



### Power Estimates under $H_{A_3}$

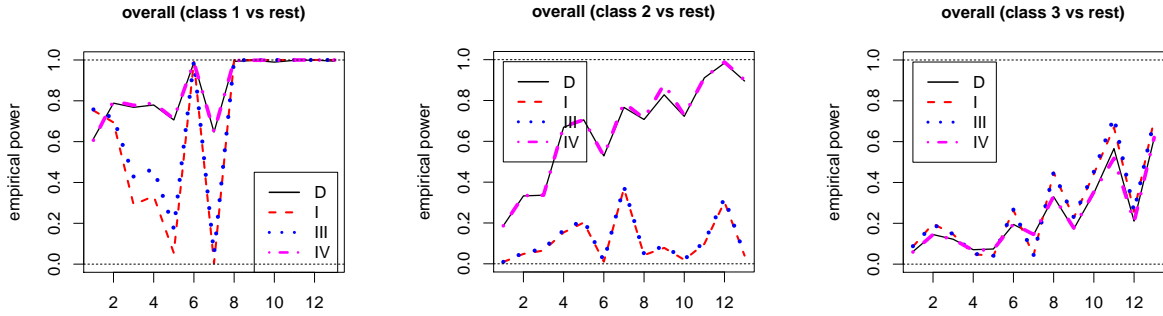


Figure 22: The empirical power estimates of the overall tests under the association alternatives  $H_{A_1}$  (top),  $H_{A_2}$  (middle), and  $H_{A_3}$  (bottom) in the three-class case with the one-versus-rest type testing. The legend labeling is as in Figure 1 and horizontal axis labels are as in Figure 4.



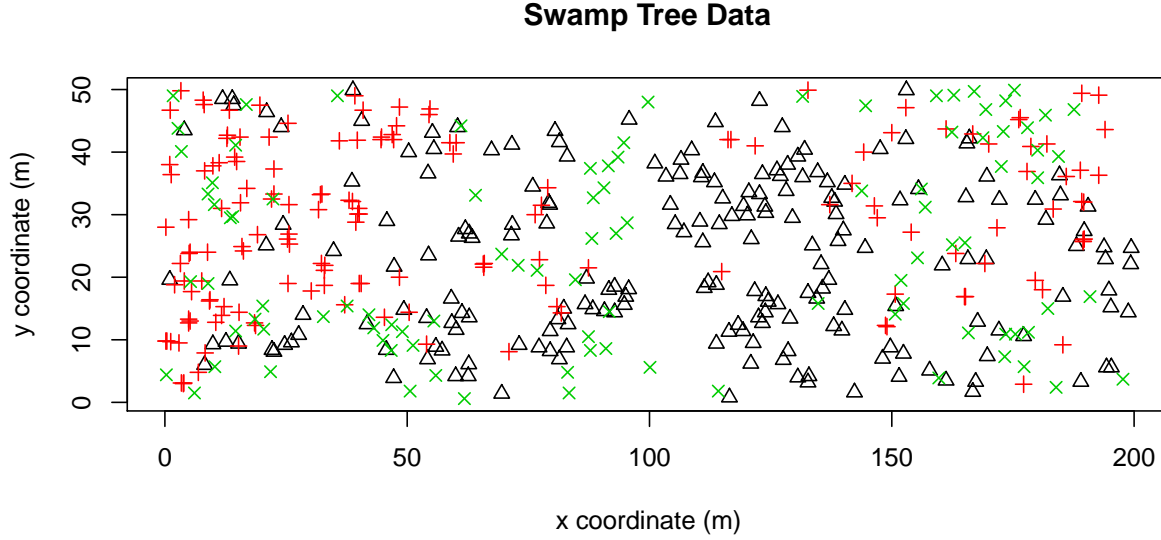


Figure 23: The scatter plot of the locations of black gum trees (triangles  $\triangle$ ), Carolina ashes (pluses  $+$ ), bald cypress trees (crosses  $\times$ ).

		NN			sum
		B.G.	C.A.	B.C.	
base	B.G.	142 (69 %)	40 (26 %)	23 (23 %)	205 (45 %)
	C.A.	34 (17 %)	98 (63 %)	25 (26 %)	156 (34 %)
	B.C.	38 (19 %)	32 (21 %)	28 (29 %)	98 (21 %)
	sum	214 (47 %)	170 (37 %)	76 (17 %)	460 (100 %)

Table 2: The NNCT for swamp tree data and the corresponding percentages (in parentheses), where the cell percentages are with respect to the size of the NN species, and marginal percentages are with respect to the total size. B.G. = black gums, C.A. = Carolina ashes, and B.C. = bald cypresses.

## 10 Example Data: Swamp Tree Data

The NNCT methodology is illustrated on an ecological data set: the swamp tree data of Good and Whipple (1982) which was also analyzed by Dixon (1994, 2002). The data set is described in detail in Ceyhan (2010). Briefly, the plot contains 13 different tree species, of which four species account for over 90 % of the 734 tree stems. In our analysis, we only consider black gums (*Nyssa sylvatica*), Carolina ashes (*Fraxinus caroliniana*), and bald cypresses (*Taxodium distichum*) (as if only these three tree species exist in the area, so we are ignoring the possible effects of other species on the spatial interaction between these species for illustrative purposes). Thus, we perform a  $3 \times 3$  NNCT-analysis on this data set. See Figure 23 for the location of the trees in this plot and Table 2 for the associated  $3 \times 3$  NNCT together with cell percentages based on NN class sizes, and marginal percentages based on the grand sum,  $n$ . When, e.g., black gum is the base species and Carolina ash is the NN species, the cell count is 40 which is 26 % of the 156 Carolina ashes (and Carolina ashes are 34 % of all trees). The percentages in Table 2 and the Figure 23 suggest that each tree species is segregated from the other trees as the observed percentages of species in the diagonal cells are much larger than the row percentages (or species percentages).

The null model in a NNCT analysis depends on the particular ecological context. Goreaud and Pélissier (2003) state that under CSR independence, the two classes are *a priori* the result of different processes (e.g., individuals of different species or age cohorts). On the other hand, under RL, some processes affect *a posteriori* the individuals of a single population (e.g., diseased vs. non-diseased individuals of a single species). Hence, in the swamp tree data, the locations of the tree species can be viewed *a priori* resulting from different processes, so the more appropriate null hypothesis is the CSR independence pattern. We compute

Overall tests					
	$C_D$	$C_I$	$C_{II}$	$C_{III}$	$C_{IV}$
	76.92	66.06	76.71	66.11	78.82
$p_{asy}$	< .0001	< .0001	< .0001	< .0001	< .0001
$p_{mc}$	< .0001	< .0001	< .0001	< .0001	< .0001
$p_{rand}$	< .0001	< .0001	< .0001	< .0001	< .0001

Table 3: Test statistics and  $p$ -values for the overall tests and the corresponding  $p$ -values.  $p_{asy}$ ,  $p_{mc}$ , and  $p_{rand}$  stand for the  $p$ -values based on the asymptotic approximation, Monte Carlo simulation, and randomization of the tests, respectively.  $C_D$  stands for Dixon’s overall test and  $C_{I-IV}$  are for types I-IV overall tests.

$Q = 282$  and  $R = 288$  for this data set and our inference will be conditional on these values. Dixon’s and the new overall segregation tests and the associated  $p$ -values are presented in Table 3, where  $p_{asy}$  stands for the  $p$ -value based on the asymptotic approximation,  $p_{mc}$  is the  $p$ -value based on 10000 Monte Carlo replication of the CSR independence pattern in the same plot and  $p_{rand}$  is based on Monte Carlo randomization of the labels on the given locations of the trees 10000 times. Notice that  $p_{asy}$ ,  $p_{mc}$ , and  $p_{rand}$  are all significant. The cell-specific test statistics and the associated  $p$ -values are presented in Table 4, where  $p$ -values are calculated as in Table 3. Again, all three  $p$ -values in Table 4 are similar for each cell-specific test.

The overall segregation tests are all highly significant which implies that there is significant deviation from the CSR independence pattern for at least one of the tree species. To determine which species exhibit segregation or association, we perform the cell-specific tests as a post-hoc analysis. At 0.05 level, Dixon’s and the new cell-specific tests agree for all cells in term of significance except for (B.C.,B.C.) cell, at which Dixon’s test is not significant but types I and III are significant. At 0.10 level tests agree for cells except (B.C.,B.G) and (C.A.,B.C.), at cell (B.C.,B.G) Dixon’s test is not significant but types I and III are significant, while at cell (C.A.,B.C.) Dixon’s test is significant but types I and III are not. At 0.01 level tests agree at cells except for cell (B.G.,B.C.) at which Dixon’s test is significant while types I and III are not. The test statistics are all positive (negative) for the diagonal (off-diagonal) cells which also support the segregation of species.

For a given class  $i$ , we estimate probabilities  $\pi_{ij}$  of Section 2.1 as  $\hat{\pi}_{ij} = N_{ij}/n_j$ . The estimated probabilities are presented in parentheses as percentages in Table 2. For example, for (B.G.,C.A.) cell,  $\hat{\pi}_{12} = N_{12}/n_2 = 40/156 \approx 0.26$ . For black gums, we have  $\hat{\pi}_{11} = 0.69 > 0.26 + 0.23$ , so black gums exhibit total segregation from the other two tree species. Similarly, for California ashes, we have  $\hat{\pi}_{22} = 0.62 > 0.17 + 0.26$ , so Carolina ashes exhibit total segregation from the other two tree species. However, bald cypresses only exhibit strong segregation, since  $\hat{\pi}_{33} = 0.29 \not> 0.19 + 0.21$ , but  $0.29 > 0.19$  and  $0.29 > 0.21$ .

We also present the one-vs-rest cell-specific and overall tests (see Table 5). For each species, we observe that the other species combined tend to be segregated from the species in consideration, but to a lesser extent for bald cypresses.

The spatial interaction is significant for each species, but at different levels. In particular, black gums exhibit significant segregation from other species (they are significantly segregated from both Carolina ashes and bald cypresses), Carolina ashes exhibit significant segregation from other species (they are significantly segregated from black gums but not from bald cypresses), and Bald cypresses exhibit significant segregation from other species (they are moderately segregated from black gums only but when the two species of black gums and Carolina ashes are considered together, the (B.C.,B.C.) cell is significant).

However, these results pertain to interaction at about the average NN distances. For the swamp tree data average NN distance ( $\pm$  standard deviation) is about 2.1 ( $\pm$  1.35) meters. We might also be interested in the possible causes of the segregation and the type and level of interaction between the tree species at different distances between the trees. Along this line, we also present the second-order analysis of the swamp tree data by the pair correlation function  $g(t)$  (Stoyan and Stoyan (1994)). The pair correlation function of a (univariate) stationary point process is defined as  $g(t) = \frac{K'(t)}{2\pi t}$  where  $K'(t)$  is the derivative of Ripley’s  $K(t)$  function. For a univariate stationary Poisson process,  $g(t) = 1$ ; values of  $g(t) > 1$  suggest clustering (or aggregation) and the values of  $g(t) < 1$  suggest inhibition (or regularity) between points. The pair correlation functions for each species are plotted in Figure 24. Black gums are aggregated for distance values of about 1-6 and 9-11 m; Carolina ashes are aggregated for all the range of the plotted distances; and bald cypresses are aggregated for distance values of about 2-8 and around 11 m. These distance ranges at which species

Dixon's cell-specific tests			
	B.G.	C.A.	B.C.
B.G.	6.60 ( $< .0001, < .0001, < .0001,$ )	-4.50 ( $< .0001, < .0001, < .0001,$ )	-3.72 (.0002, $< .0001, .0005$ )
C.A.	-5.69 ( $< .0001, < .0001, < .0001$ )	6.64 ( $< .0001, < .0001, < .0001$ )	-1.72 (.0846, .0855, .0846)
B.C.	-1.16 (.2469, .2773, .2406)	-0.33 (.7445, .7539, .7284)	1.52 (.1292, .1228, .1402)
Type I cell-specific tests			
	B.G.	C.A.	B.C.
B.G.	6.94 ( $< .0001, < .0001, < .0001$ )	-6.33 ( $< .0001, < .0001, < .0001$ )	-2.36 (.0185, .0176, .0189)
C.A.	-6.90 ( $< .0001, < .0001, < .0001$ )	6.54 ( $< .0001, < .0001, < .0001$ )	-0.23 (.8158, .8153, .8137)
B.C.	-1.65 (.0986, .1000, .0933)	-0.99 (.3234, .3251, .3285)	2.62 (.0089, .0085, .0082)
Type III cell-specific tests			
	B.G.	C.A.	B.C.
B.G.	6.94 ( $< .0001, < .0001, < .0001$ )	-6.33 ( $< .0001, < .0001, < .0001$ )	-2.35 (.0187, .0179, .0192)
C.A.	-6.90 ( $< .0001, < .0001, < .0001$ )	6.54 ( $< .0001, < .0001, < .0001$ )	-0.23 (.8187, .8225, .8174)
B.C.	-1.65 (.0984, .0999, .0933)	-0.99 (.3228, .3250, .3283)	2.61 (.0091, .0087, .0083)

Table 4: Test statistics and  $p$ -values for the cell-specific tests and the corresponding  $p$ -values (in parentheses). The  $p$ -values are given in the order of  $p_{asy}$ ,  $p_{mc}$ , and  $p_{rand}$ , whose labeling is as in Table 3. B.G. = black gums, C.A. = Carolina ashes, and B.C. = bald cypresses.

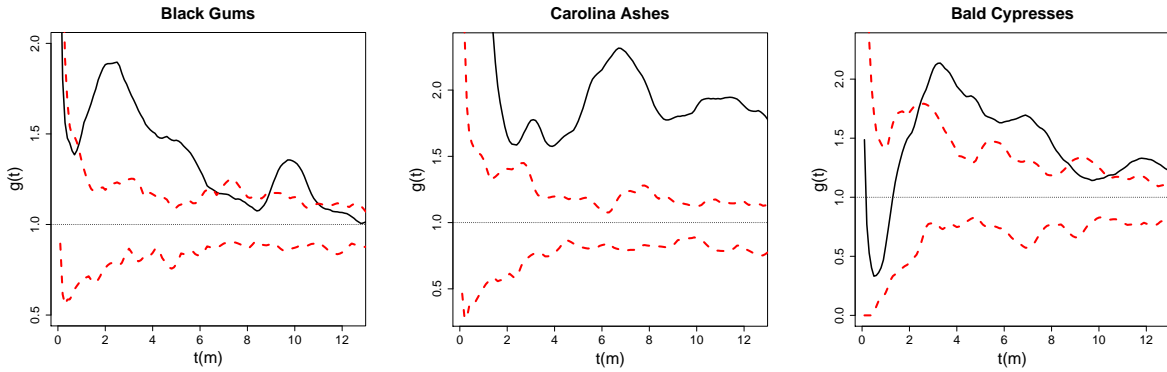


Figure 24: Pair correlation functions for each species in the swamp tree data. Wide dashed lines around 1 (which is the theoretical value) are the upper and lower (pointwise) 95 % confidence bounds for the pair correlation functions based on Monte Carlo simulation under the CSR independence pattern.

One-vs-rest Cell-specific Tests			
	$Z_{22}^D$	$Z_{22}^I$	$Z_{22}^{III}$
B.G.-vs-rest	5.11 (< .0001)	6.94 (< .0001)	6.93 (< .0001)
C.A.-vs-rest	3.91 (< .0001)	6.54 (< .0001)	6.54 (< .0001)
B.C.-vs-rest	4.13 (< .0001)	2.62 (.0044)	2.62 (.0044)

One-vs-rest Overall Tests					
	$C_D$	$C_I$	$C_{II}$	$C_{III}$	$C_{IV}$
B.G.-vs-rest	49.27 < .0001	48.09 < .0001	49.27 < .0001	48.09 < .0001	49.27 < .0001
C.A.-vs-rest	44.84 < .0001	42.74 < .0001	44.84 < .0001	42.78 < .0001	45.44 < .0001
B.C.-vs-rest	17.05 .0002	6.84 .0089	17.04 .0002	6.90 .0086	17.03 .0002

Table 5: Test statistics and  $p$ -values for one-vs-rest cell-specific tests for cell (2, 2) (the corresponding  $p$ -values are presented in parenthesis) and one-vs-rest overall tests (the corresponding  $p$ -values are presented below the test statistics).  $Z_{22}^D$  stands for Dixon's cell-specific test, and  $Z_{22}^I$  and  $Z_{22}^{III}$  stand for type I and III cell-specific tests.  $C_D$  stands for Dixon's overall test and  $C_{I-IV}$  are for types I-IV overall tests.

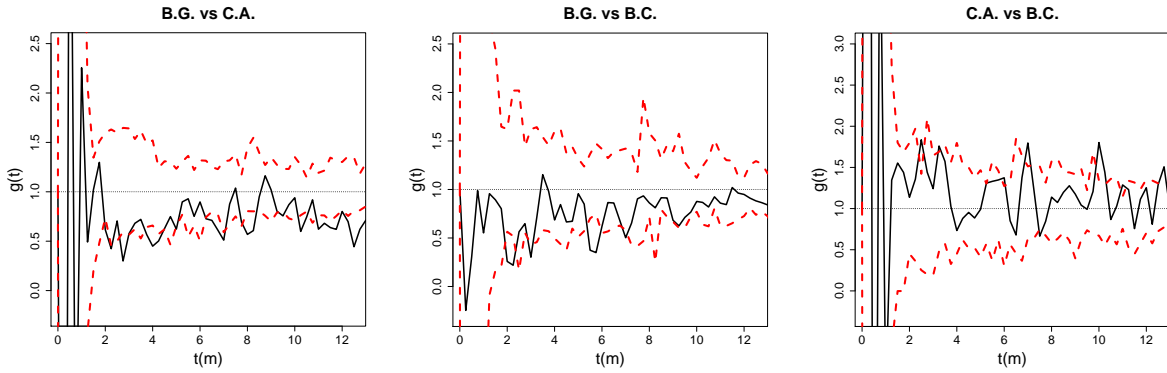


Figure 25: Pair correlation functions for each pair of species in the swamp tree data. Wide dashed lines around 1 (which is the theoretical value) are the upper and lower (pointwise) 95 % confidence bounds for the pair correlation functions based on Monte Carlo simulations under the CSR independence pattern. B.G. = black gums, C.A. = Carolina ashes, and B.C. = bald cypresses.

are aggregated include the mean NN distance for our data, hence this aggregation could be the reason of the significant segregation between the species.

The same definition of the pair correlation function can be applied to Ripley's bivariate  $K$  or  $L$ -functions. Under CSR independence we have  $g(t) = 1$ ;  $g(t) > 1$  suggests association of the classes; and  $g(t) < 1$  suggests segregation of the classes. The bivariate pair correlation functions for the species in swamp tree data are plotted in Figure 25. Black gums and Carolina ashes are segregated for about 2-2.5, 3.5-4.5, 7.5-8.5, and 10.5-12 m; black gums and bald cypresses are segregated for about 2.5, 3, and 6 m; and Carolina ashes and bald cypresses are associated for 7 and 9 m.

The pair correlation function estimates have considerably high variability for small  $t$  if  $g(t) > 0$ , hence not so reliable for small distances (Stoyan and Stoyan (1996)). See for example Figures 24 and 25 where the confidence bands for small  $t$  values are much wider compared to those for larger  $t$  values. So pair correlation function analysis is more reliable for larger distances, say, larger than about the average NN distance in the data set. While the pair correlation function provides information on the univariate and bivariate patterns at all distances, NNCT-tests summarize the spatial interaction for distances about the average NN distance in the data set.

## 11 Discussion and Conclusions

We introduce cell-specific and overall segregation tests based on nearest neighbor contingency tables (NNCTs). NNCT-tests are used in testing randomness in the nearest neighbor (NN) structure between two or more classes. The overall test is used for testing any deviation from randomness in all the NNCT cells combined; cell-specific test for cell  $(i, j)$  is used for testing any deviation from randomness in cell  $(i, j)$ , i.e., NN structure in which base class is  $i$  and NN class is  $j$ . This statistic tests the segregation or lack of it, if  $i = j$ ; the association or lack of it between classes  $i$  and  $j$ , if  $i \neq j$ . The randomness in the NN structure is implied by the RL or CSR independence patterns. We demonstrate that under the CSR independence pattern, NNCT-tests are conditional on  $Q$  and  $R$ , while under the RL pattern, these tests are unconditional. In the two-class case, cell-specific tests are essentially different only for two cells, since cell  $(1, 1)$  and  $(1, 2)$  yield the same test statistic in absolute value for Dixon's cell-specific test, likewise for cells  $(2, 1)$  and  $(2, 2)$ . Similarly, cell  $(1, 1)$  and  $(2, 1)$  yield the same test statistic in absolute value for the type III cell-specific test, likewise for cells  $(1, 2)$  and  $(2, 2)$ . For type I cell-specific test cells  $(1, 1)$  and  $(2, 2)$  yield the same test statistic, and the off-diagonal cells give the negative of this value.

We demonstrate that the cell-specific tests tend to standard normal distribution, as the sample size gets larger. On the other hand, the overall tests tend to chi-square distribution with the corresponding degrees of freedom with the increasing sample size. Two major types of asymptotic structures for spatial data exist in literature: infill asymptotics and increasing domain asymptotics (Lahiri (1996)). In "infill asymptotics" the region of interest is a fixed bounded region and the number of observed points gets larger in this region. Hence the minimum distance between data points tends to zero as the sample size tends to infinity. In "increasing domain asymptotics", any two observations are required to be at least a fixed distance apart, hence as the number of observations increase, the region on which the process is observed eventually becomes unbounded (Cressie (1993)). The sampling structure in our asymptotic sampling distribution could be either one of these asymptotic structures. Because we only consider the class sizes and hence the total sample size tending to infinity regardless of the size of the study region.

Based on our Monte Carlo simulations, we observe that the asymptotic approximation for the cell-specific tests is appropriate only when the corresponding cell count in the NNCT is larger than 10; and for the overall test when all cell counts are at least 5. For NNCTs with smaller cell counts, we recommend the Monte Carlo randomization of the tests. In the two-class case, types I and III cell-specific tests have better empirical size performance for the cell corresponding to the smaller sample, while Dixon's cell-specific test has better size performance for the cell corresponding to the larger sample. For the overall test, the performance of the cell-specific tests are similar for Dixon's and types I and III tests, all of which have better performance compared to type IV test. In the three class case, types I and III cell-specific tests have better size performance, and type III overall test have better size performance. We also observe that types I and III cell-specific tests and type III overall test are more robust to the differences in sample sizes (i.e., differences in relative abundance). Under the *segregation alternatives*, in the two-class case, types I and III cell-specific tests have similar power estimates which are larger than those of Dixon's, and for the overall tests, types I and III overall tests have higher power estimates for large sample size combinations. In the three class case, types I and III cell-specific tests have higher power estimates, while for the overall tests, type III test has higher power estimates. Under the *association alternatives*, in the two-class case, types I and III cell-specific tests (Dixon's cell-specific tests) have higher power estimates for the class with the smaller (larger) sample size, and for the overall tests, types I and III overall tests have higher power estimates for large sample size combinations. In the three class case, types I and III cell-specific tests have higher power estimates for cell  $(i, j)$  if  $n_i$  is less than  $n_j$ , while Dixon's cell-specific tests have higher power estimates if  $n_i$  is larger than  $n_j$ . For the overall tests, Dixon's overall test has the highest power estimates. When empirical size and power performances are considered together, among cell-specific tests, types I and III cell-specific tests are recommended against the segregation alternatives, while types I, III, and Dixon's cell-specific test are recommended against the association alternatives. Among overall tests, type III overall tests are recommended against the segregation alternatives, while Dixon's overall test is recommended against the association alternatives.

NNCT-tests summarize the pattern in the data set for small scales around the average NN distance between all points. On the other hand, pair correlation function  $g(t)$  and Ripley's classical  $K$  or  $L$ -functions and other variants (Baddeley et al. (2000)) provide information on the pattern at various scales (i.e., around other distance values). Hence NNCT-tests and pair correlation or  $K$ -functions are not comparable but provide complimentary information about the pattern in question. However, an advantage of overall NNCT-tests is

that they provide the interaction in a multi-class setting in the presence of all classes, while the second order analysis with  $K$  or  $g$  functions allow a comparison of pairs of classes (one at a time). Furthermore, when an overall NNCT-test is significant, it offers various post-hoc tests to follow up the specifics of the interaction: (i) cell-specific tests, (ii) one-class-vs-rest type tests, and (iii) class-specific tests. In the cell-specific tests for cell  $(i, j)$ , the interaction between classes  $i$  and  $j$  are examined in the presence of all other classes, and in the class  $i$ -vs-rest testing, the interaction of all the classes other than class  $i$  with class  $i$  is investigated. The pair correlation function and  $K$ -functions can also be adapted for one-vs-rest type analysis, as classes  $i$  and the rest of the classes can be treated as the two classes we use our analysis.

The course of action we recommend depends on which null hypothesis is more appropriate. If CSR independence is the reasonable null pattern, we recommend the overall segregation test to detect the spatial interaction at small scales at about the mean NN distance. If it yields a significant result, then to determine which pairs of classes have significant spatial interaction, the cell-specific tests or one-vs-rest type tests can be performed (we recommend both versions as they provide information on different aspects of the spatial interaction). To detect spatial interaction at larger distances, pair correlation function is recommended (Stoyan and Penttinen (2000)), due to the cumulative nature of Ripley's  $K$ - or  $L$ -functions for larger distances. On the other hand, if the RL pattern is the reasonable null pattern, we recommend the NNCT-tests to detect the interaction at about the mean NN distance, and Diggle's  $D$ -function (Diggle (2003)) or modified version of Ripley's  $K$  function (Baddeley et al. (2000)) to detect the interaction at higher distances.

## Acknowledgments

Most of the Monte Carlo simulations presented in this article were executed at Koç University High Performance Computing Laboratory.

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